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$E(Kl_3m_{4,5})$ and $E(L_3m_xm_{4,5})$ Auger Electron Kinetic Energiesfor $21 \leq Z \leq 30$

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Abstract
This paper describes the work on the calculation of the $KL_3M_{4,5}$ and$L_3M_XM_{4,5}$ Auger electron kinetic energies for the atomic numbers Z= 21 to 30. These energyvalues are calculated using themethod of screening and are presented here for the first time.

Keywords: *Auger electron, transitions, doublyionized atoms,vacancies,levelbinding energy.*

I. INTRODUCTION

when highly energetic electrons strike with the target of anx-ray tube, x-rays are produced due to the impact of the electron. Now if thesex-rays are absorbed by material itself,further vacancies are created in the atom.When a K-electron is ejected from the atom, a vacancy is created in the K-shell and if,consequently itis filled by the L-shell electron and after the transition from
L-shell to the K-shell, the energy emitted in the form of electromagnetic radiation is absorbed by the emitting atom itself, another electron is ejected and the atom finally becomes doubly ionized.

This process is known as Augerprocess (1923,1925)[1-2] and the ejected electron is known as Auger electron. In this process no electro-magnetic radiation is emitted from the atom, so it is an internal conversion process and is also known as aradiationless process.

The low atomic number elements show better Auger effect than the high atomic number elements. If one of these double vacanciesare filled by an electron from higher energy shell, x-ray satellites are produced.

The study of theseAuger electrons is broadly covered in the field of "Auger Electron Spectroscopy"[3]which plays very important role in investigations carried out by Scientists and Engineers alike. Scientists utilizes these studies for exploring atomic structure,elemental analysis and chemical problems etc. whereas the studies on surfaces of materials play vital role in the era of Engineering and Technology. It is very well established that the use of Auger electron kinetic energies is the backbone of all these studies.

Larkins (1977)[4] using the relativistic Hartee-Fock-Slater formulism has calculated all possible Auger transitions and their energies for the elements $10 \leq Z \leq 100$. This table is the only available comprehensive source for the Auger

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electron kinetic energies. A scrutiny of these tables reveals that these Auger electron kinetic energies for the $KL_3M_{4,5}$and $L_3M_XM_{4,5}$transitions are known only for the atomic number 30 in the atomic number range Z= 21 – 30 (Larkins 1977[4]). Neither such values for Z= 21 to 29 are reported by Larkins (1977)[4]in his compilation nor any such experimental results are reported elsewhere and hence their calculation using even simplest method becomes of critical significance.Our future interest involves systematization and exploring the origin of theLα x-ray satellites for the atomic number range z= 21- 30 which also requires $KL_3M_{4,5}$ and $L_3M_XM_{4,5}$Auger electron kinetic energies.

In this paper we are interested in the calculation of these Auger electron kinetic energies for the transitions $KL_3M_{4,5}$ and $L_3M_XM_{4,5}$ where X = 1 to 5 for the atomic number range Z=21 to 30.

II. METHODOF CALCULATION

The desired Auger electron kinetic energy valuesE($KL_3M_{4,5}$) andE($L_3M_XM_{4,5}$) can be calculated using the following well known equations:

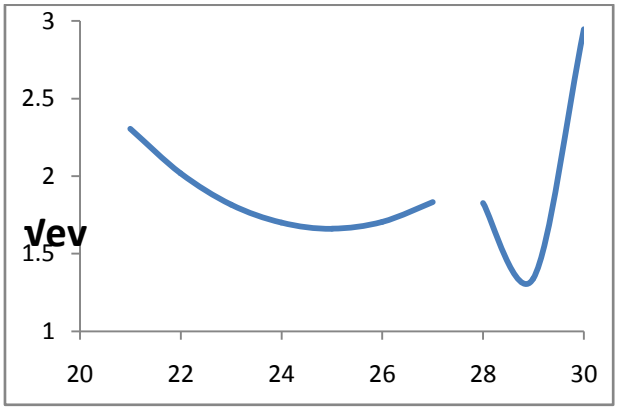
$$\mathbf{E(KL_3M_{4,5}) = E(K)_Z - E(L_3)_Z - E(M_{4,5})_{Z+\Delta Z}} \quad \mathbf{(1)}$$

$$\mathbf{E(L_3M_XM_{4,5}) = E(L_3)_Z - E(M_X)_Z - E(M_{4,5})_{Z+\Delta Z'}} \quad \mathbf{(2)}$$

Where the symbols have their usual meaning and ΔZ, ΔZ' signifies the increased nuclear pull (Burhop and Assad1972[5]) on the level $M_{4,5}$due to the additional vacancy in the L_3 and M_X shells respectively.

The L_3 and K level binding energy values used in these calculations are taken from Bearden and Burr compilation(1967)[6], $E(M_X)_Z$, where x=1 to 3 is taken from Bearden and Burr table[6] and the $M_4$and M_5 level binding energies from the resolved energy values ofMisraet al. (1992)[7].The energy values $E(M_{4,5})_{Z+\Delta Z}$ and $E(M_{4,5})_{Z+\Delta Z'}$ are calculated using the procedure given below.

The precise resolved energy values for M_4 and M_5 levels, taken from Misra et al. (1992)[7], are used to plot the Mosley diagram.This graph does not emerge to be a straight line as expectedbut showsdiscontinuous parabolic behaviour between Z= 27 and Z = 28 figure(1).



Figure(1) Mosley plot for the resolved energy values $E(M_4)$ for Z=21-30

Therefore separate plots are drawn for Z=21 to 27 and for Z= 28 to 30.
The shapes of both of these graphsare parabolic and i.e. for Z=21 to 27 as well as for Z= 28 to30 and asecond order Polynomial is fitted to the curves so obtained. The equation of the curve for the level M_4 in the atomic number range Z= 28 – 30 becomes:

$$\sqrt{ev} = \mathbf{1.0455Z^2 – 60.079Z + 864.38} \quad \mathbf{(3)}$$

where $\sqrt{ev}$is the square root of the M_4 level energy and Z is the atomic number.

The Auger electron kinetic energy values for various $KL_3M_{4,5}$ and $L_3MxM_{4,5}$ transitions for Z=30 are known from Larkins (1977) wherefrom energies $E(M_{4,5})_{Z+\Delta Z}$ and $E(M_{4,5})_{Z+\Delta Z'}$ for various $^{2s+1}L_j$ levels can be obtained using the equations 1 and 2.After putting the square root of the so obtained energy value for Z=30 for the $E(M_{4,5})_{Z+\Delta Z}$and $E(M_{4,5})_{Z+\Delta Z'}$ in the above quadratic equation and solving it for Z using formula

$$Z = \frac{-B \pm \sqrt{B^2-4AC}}{2A}$$

whichis solution for the equation $AZ^2 + bZ + C = 0$

We get two values for Z and the positive value is considered by which the corresponding incremented new atomic number (Z+ΔZ) and (Z+ΔZ') satisfying the equation is obtained for Z= 30. This makes it possible to calculate ΔZ and ΔZ' for Z= 30 for any configuration $^{2s+1}L_j$ in presence of an additional vacancy in the L_3 and M_X level.

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Similarly to get the ΔZ, ΔZ' and finally the energy values for the atomic number range Z= 21 to 27 for the M_4 level,the Mosley plot equation is found to satisfy the equation:

$$\sqrt{ev} = 0.0411Z^2 - 2.0521Z + 27.265 \quad (4)$$

For the M_5level in the atomic number range Z= 28 to 30, the equation for the Mosley plot is:

$$\sqrt{ev} = 1.045Z^2 - 60.048Z + 863.85 \quad (5)$$

To obtain the ΔZ, ΔZ' and finally the energy values for atomic number range 21 to 27 for M_5level, the equation for the Mosley plot becomes:

$$\sqrt{ev} = 0.041Z^2 - 2.0495Z + 27.218 \quad (6)$$

It is very well explained by many authors (Sommerfeld 1934[8],Burns 1964[9], Slater1960[10]) that the behavior of the Moseley plot for level energy$E(M_x)_{Z+\Delta Z}$ will be same as for $E(M_x)_Z$. Further the increment (ΔZ) and (ΔZ') for a level $^{2s+1}L_j$ will be uniform and the same for the entire series i.e. for Z= 21 to 30. Now putting the value Z+ΔZ and Z+ΔZ', so obtained from the data for Z=30, in the above equations, one can obtain the corresponding energy values for Z= 21 - 30 for the various $E(M_{4,5})_{Z+\Delta Z}$ and $E(M_{4,5})_{Z+\Delta Z'}{}^{2s+1}L_j$ levels.

III. RESULTSAND DISCUSSION

The table 1 showsall the allowed Auger electron kinetic energy values so calculated for $E(KL_3M_{4,5})$for the atomic number range Z= 21 to 30 whereas table 2 contains all such calculated energy values for$E(L_3M_XM_{4,5})$. It must be pointed out that all these energy values are calculated for the first time.

Although numerous final configurations emerge after coupling of levels $L_3M_{4,5}$and $M_xM_{4,5}$but the ones permitted by well known Pauli exclusion principle(Condon and Shortley 1935[12], White 1934[13]) and adopted by Larkins[4] for his work,are only taken into consideration for such calculations.

These calculations consider existence of electrons in both the M_4 andM_5 levels in the atomic number range 21-30, where presence of electrons in both the $3d_{3/2}d_{5/2}$ levels is doubtful especially for low Z values in this range. But the existence of experimental data on the $L\alpha_{1,2}$ x-ray diagram line i.e. L_3-M_4 and L_3-M_5 transitions (Cauchois and Senemaud 1978[14]), fully rules out any such doubt and allows us to proceed further for such calculations. TheseAuger electron kinetic energyvaluesare calculated usingvery approximate and simple method of screening (Compton and Allison 1935[11], Burhop and Assad 1972[5], Sommerfeld 1934[8]),therefore one should not expect very high accuracy in these results. Butwe know that non-availability of such data lead nowhere and the atomic processes involving these valuescan not beunderstood properly. This definitely makes our results very fruitful for further investigations.

V. CONCLUSION

A very simple method based on screening was successfully developed to obtain theAuger electron kinetic energieswhichmight not have succeeded in achieving very accurate results.Therefore very accurate quantum mechanical calculations and precise experimental measurements of these kinetic energies are an absolute demand of the hour and this will certainly lead to precise understanding of various atomic processes in this low atomic number region.

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Table 1

At.No.	Auger Electron Kinetic Energy (eV)						
	$E(KL_3M_4, {}^3P_0)$	$E(KL_3M_4, {}^1P1)$	$E(KL_3M_4, {}^3D_2)$	$E(KL_3M_4, {}^1F_3)$	$E(KL_3M_5, {}^3P_1)$	$E(KL_3M_5, {}^3D_3)$	$E(KL_3M_5, {}^3F_4)$
21	4085.98	4086.04	4085.96	4086.02	4086.15	4086.10	4086.08
22	4507.28	4507.32	4507.26	4507.30	4507.43	4507.40	4507.38
23	4949.17	4949.19	4949.16	4949.18	4949.31	4949.30	4949.29
24	5411.95	5411.95	5411.94	5411.95	5412.09	5412.08	5412.08
25	5895.94	5895.93	5895.94	5895.94	5896.09	5896.09	5896.10
26	6400.86	6400.84	6400.86	6400.84	6401.02	6401.04	6401.04
27	6926.65	6926.61	6926.66	6926.63	6926.84	6926.86	6926.88
28	7476.29	7476.35	7476.26	7476.33	7476.44	7476.38	7476.35
29	8044.32	8044.02	8044.44	8044.14	8044.45	8044.68	8044.78
30	8618.60	8617.20	8619.30	8617.70	8618.90	8620.10	8620.80

Table 2

At.No.	Auger Electron Kinetic Energy (eV)										
	$E(L_3M_3M_4, {}^3D_3)$	$E(L_3M_3M_4, {}^3F_2)$	$E(L_3M_4M_4, {}^3P_2)$	$E(L_3M_3M_4, {}^3D_1)$	$E(L_3M_4M_5, {}^3P_1)$	$E(L_3M_1M_5, {}^3D_3)$	$E(L_3M_5M_5, {}^3P_0)$	$E(L_3M_5M_5, {}^3F_4)$	$E(L_3M_1M_4, {}^3D_1)$	$E(L_3M_5M_5, {}^3F2)$	$E(L_3M_4M_4, {}^1S_0)$
21	365.7	365.45	392.13	365.7	392.3	343.85	392.45	392.45	343.67	392.32	392.36
22	417.16	417	447.71	417.16	447.86	391.67	447.98	447.98	391.5	447.9	447.85
23	471.7	471.61	506.52	471.7	506.67	443.48	506.77	506.77	443.33	506.73	506.60
24	529.44	529.41	568.84	529.44	568.98	497.78	569.09	569.09	497.63	569.07	568.86
2	590.35	590.37	634.8	590.35	634.94	553.8	635.05	635.05	553.65	635.06	634.77

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5											
26	652.15	652.23	702.19	652.15	702.35	612.35	702.46	702.46	612.19	702.5	702.11
27	715.38	715.52	771.68	715.38	771.86	674.49	771.98	771.98	674.32	772.05	771.54
28	786.61	786.21	849.35	786.61	849.52	741.12	849.69	849.69	740.93	849.46	849.63
29	854.69	855.57	926.39	854.69	926.52	808.38	926.57	926.57	808.3	926.98	925.39
30	913.91	919.3	994.2	913.91	994.2	866.4	994.2	994.2	866.4	996.9	988.40

Table 2(CONTINUED)

At.No.	**Auger Electron Kinetic Energy (eV)**									
	$E(L_3M_4M_5,^1G_4)$	**$E(L_3M_1M_5,^3D_2)$**	**$E(L_3M_2M_4,^3D_2)$**	**$E(L_3M_3M_5,^3P_1)$**	**$E(L_3M_4M_5,^3F_3)$**	**$E(L_3M_4M_5,^1D_2)$**	**$E(L_3M_2M_5,^3P_2)$**	**$E(L_3M_3M_5,^1D_2)$**	**$E(L_3M_3M_5,^3F_4)$**	**$E(L_3M_3M_4,^3P_0)$**
21	392.34	343.84	365.17	365.85	392.17	392.29	365.3	365.58	365.58	365.66
22	447.89	391.66	416.53	417.3	447.78	447.86	416.66	417.12	417.12	417.13
23	506.68	443.48	470.94	471.83	506.62	506.66	471.07	471.73	471.73	471.68
24	568.99	497.77	528.52	529.58	568.96	568.98	528.65	529.55	529.55	529.44
25	634.94	553.8	589.22	590.5	634.95	634.94	589.37	590.52	590.52	590.36
26	702.34	612.36	650.75	652.32	702.39	702.36	650.93	652.4	652.4	652.16
27	771.83	674.5	713.69	715.58	771.93	771.86	713.9	715.73	715.73	715.4
28	849.58	741.1	784.3	786.74	849.28	849.5	784.4	786.28	786.28	786.56
29	926.38	808.42	852.76	854.93	926.92	926.56	853.01	855.83	855.83	854.86
30	993.62	866.4	913.9	914.7	996.9	994.7	914.7	920.2	920.2	914.7