NOTE

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An additive property of Slater's screening constants with reference to X-ray *K*-emission lines

Amar Nath Nigam* and Sanjay Kumar Srivastava
Physics Department, Harcourt Butler Technological Institute, Kanpur 208 002, India

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Abstract : The Mosley plots for X-ray *K*-satellite lines show an interesting feature. The screening for the $K\alpha_1$ satellites is lesser than that for the parent line $K\alpha_1$. The case for the satellites of $K\beta_1$ is just the reverse. It is shown that this can be accounted for by suitably adding the Slater screening values for the initial and final configurations arising out of the double ionisation.

Keywords : Screening constants, X-ray satellite lines, double ionisation

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Our objective behind putting this note is to point out that Slater's screening constants can be used additively to obtain the screening shown by the X-ray *K*-lines. Table 1 below shows this property.

Table 1. Additivity of Slater's screening constant for $K\alpha$ and $K\beta$ diagram lines

Line and transition		Screening obtained from Mosley plots	Screening obtained by adding Slater's screening constants	
$K\alpha_1$	KL_{III} }	1.13	$\sigma_{1s} + \sigma_{2p} = 0.3 + 0.85$	$= 1.15$
$K\alpha_2$	KL_{II} }			
$K\beta_{1,3}$	$KM_{III,II}$	2.0	$\sigma_{1s} + \sigma_{3p} = 1 + 0.85$	$= 1.85$
$K\beta_2$	$KM_{IV,V}$	2.5	$\sigma_{1s} + \sigma_{3p} = 1 + 1$	$= 2$

The $K\beta_{2,5}$ line is a faint and a broad line. It is not purely an atomic transition because its features are greatly influenced by the solid state effects. Hence,there is a discrepancy in observed and estimated values of σ. Here the following values of σ have been used for different subshells (Slater 1930, 1955, 1960;Agarwal 1979)

$$\begin{aligned} \sigma_{1s} &= 0.3 & \sigma_{3s} &= 0.35 \\ \sigma_{2s} &= 0.35 & \sigma_{3p} &= 0.85 \\ \sigma_{2p} &= 0.85 & \sigma_{3d} &= 1 \end{aligned} \quad (1)$$

* Present address : 8/20 Arya Nagar, Kanpur.

For $n = 1$, the above values hold good but for $n > 2$, σ_{1s} is taken as 1. These are Slater's rules.

As such there is no theory to predict the screenings obtained for X-ray lines, only the Mosley plots yield the screening values. It is seen that the screening of an X-ray K-line is obtained by adding Slater's screening* for the missing electron. The authors have no theoretical explanation for this result at present. The advantage of this empirical result is that if accepted it can account for certain features of the K X-ray satellites which are otherwise not explicable.

The X-ray satellites arise out of double ionisation in the inner shells. Therefore, the screening shown by the Mosley plot of these satellites should be less than that of the parent line. This holds true for the $K\alpha$ satellites but not for the satellites of $K\beta_1$. The present method of adding Slater's screening for the missing electrons accounts for this fact as will be shown below. We first justify the use of Mosley law for X-ray satellites.

Justification for using Mosley law for X-ray satellites :

An atom, doubly-ionised in the inner shells is a He-like atom, in which one electron is in the ground state which the other one is in the excited. The initial states for $K\alpha$ satellites have configuration ($1s$, $2p$), ($1s$, $2s$) etc. Such He-like levels can be approximated according to Bethe and Salpeter (1957) by

$$E_{n,l,j} = -\frac{Z^2}{2} - \frac{(Z-1)^2}{n^2} \tag{2}$$

and will, therefore, obey the Mosley law. The final states have both the electrons in the excited levels. Analytical expressions for such states in L-S coupling are not to be found but in j-j coupling. Candlin (1955) writes for a level,

$$\text{Energy value} = \text{a term proportional to } Z^2 - \sigma^2$$
$$+ \text{ a relativistic term} + \text{a minor term in } Z \tag{3}$$

Replacing $Z^2 - \sigma^2$ by $(Z - \sigma)^2$ has a small error (about 10-15% in $Z = 20 - 30$ range). Thus the Mosley law holds for both initial and final states.

The $K\alpha$ satellites :

Data on υ / R values for various $K\alpha$ satellites were taken from the paper by Deodhar and Padalia (1963) and also from Deodhar (1931), Wetterbald (1927), Randall and Parratt (1940), Shaw and Parratt (1936). The Mosley graph fitting was done using a computer programme. Table 2 collects the data indicating the transitions assigned by Kenard and Ramberg (1934). These authors do not regard $K\alpha''_3$ as an emission between to doubly ionised states. This line

*Sommerfeld's σ_1 are not additive :

$$(\sigma_1)_{K\alpha_{1,2}} \neq (\sigma_1)_{K_{edge}} + (\sigma_1)_{L_{II,III\ edge}}$$

Table 2. Calculation of the screening constants for $K\alpha$ satellites as described in the text

Line	Initial state		σ_i	Final state		σ_f	$\sigma = \sigma_i + \sigma_f$	Observed σ
$K\alpha_4$	$1s\,2p$	^1P	$(\sigma_{1s} + \sigma_{2p} - 2\sigma_{2s})$ $= 0.3 + 0.85 - 0.7$ $= 0.45$	$2p\,2p$	^1D	$(2\sigma_{2p} - 2\sigma_{2s} - 2\sigma_{2s})$ $= 1.7 - 0.7 - 0.6$ $= 0.4$	0.85	0.864
$K\alpha'_3$	$1s\,2s$	^3S	$(\sigma_{1s} + \sigma_{2s} - \sigma_{2s})$ $= 0.3 + 0.35 - 0.35$ $= 0.3$	$2s\,2p$	^3P	$(\sigma_{2s} + \sigma_{2p} - 2\sigma_{2s})$ $= 0.35 + 0.85 - 0.7$ $= 0.5$	0.80	0.910
$K\alpha_3$	$1s\,2p$	^3P	0.45	$2p\,2p$	^3P	0.4	0.85	0.877
$K\alpha'$	$1s\,2p$	^1P	0.45	$2p\,2p$	^1P	0.4	0.85	1.052
$K\alpha''$	$1s\,2s$	^1S	0.3	$2s\,2p$	^1P	0.5	0.80	0.722

Table 3. Estimation of σ for $K\beta$ satellites.

Line	Initial state	σ_i	Final state	σ_f	$\sigma = \sigma_i + \sigma_f$	Observed σ
			Data from Deodhar and Padalia (1962)			
$K\beta_7$	$KM_{II,III}$	$(\sigma_{1s} + \sigma_{3p} - 2\sigma_{3s})$	M_{III}^2	$2\sigma_{3p} - 2\sigma_{3s}$		
		$1 + 0.85 - 0.7 = 1.15$		$2 \times 0.85 - 2 \times 0.35 = 1$	2.15	2.91
$K\beta_6$	KL_I	$\sigma_{1s} + \sigma_{2s}$	$L_I M_{II}$	$\sigma_{2s} + \sigma_{3p} - 2\sigma_{3s}$		
		$1 + 0.35 = 1.35$		$0.35 + 0.85 - 2 \times 0.35 = 0.5$	1.85	2.00
$K\beta_4$	$KL_{II,III}$	$\sigma_{1s} + \sigma_{2p} - 2\sigma_{2s}$	$L_{III}M_{III}$	$\sigma_{2p} + \sigma_{3p} - 2\sigma_{3s}$		
		$1 + 0.85 - 0.7 = 1.15$		$0.85 + 0.85 - 0.7 = 1.0$	2.15	2.80
$K\beta_8$	KL_I	1.35	$L_I M_{III}$	0.5	1.85	2.60
			Data from Cauchois and Senemaud (1978)			
$K\beta_{10}$	KM_I	$\sigma_{1s} + \sigma_{3s}$	$M_I M_{II,III}$	$\sigma_{3s} + \sigma_{3p}$		
		$1 + 0.35 = 1.35$		$0.35 + 0.85 = 1.2$	2.55	2.30
$K\beta_7$	$KM_{II,III}$	$\sigma_{1s} + \sigma_{2p} - 2\sigma_{3s}$	$M_I M_{IV,V}$	$\sigma_{3s} + \sigma_{3d}$		
		$1 + 0.85 - 2 \times 0.35 = 1.15$		$0.35 + 0.85 = 1.2$	2.35	2.30
$K\beta_6$	$KL_{II,III}$	1.15	$L_{II,III}M_{II,III}$	1.0	2.15	3.30
$K\beta_8$	The same as above					

has not been included in the present calculation. Also included in this table are calculations for σ using the above method. These σ values are compared with the observed values obtained by Mosley law after a computer fitting of the data was made.

It may be remarked that $1s\ 2s$ has states ^1S, ^1P and ^3S. The wave function of these states will be different but the present empirical method does not take into account this difference. This is a limitation of this method. For better results two-electron wave functions should be used in eq. (3).

The Kβ satellites :

Data on $K\beta$ satellites were collected from two sources : Deodhar and Padalia (1962) and wavelength tables of Cauchois and Senemaud (1978). The later authors quote a reference due to Sawada (1932) who assigned transitions to some of the satellites using a different nomenclature but the lines could identified from their υ / R values. Table 3 collects data for $K\beta$ satellites and its arrangement is similar to that of Table 2.

A possible interpretation of the empirical method :

In the case of double ionisation satellites it is customary to consider the atom with atomic number $Z + 1$ which is regarded as the effective nuclear charge, created by the absence of $1s^1$ electron or better called as the K-hole. If the screening due to $1s$ electron is 0.3 in Slater's scheme, its absence should raise the nuclear charge by 0.3 instead of 1. For a vacancy in $1s$ $2s$ the nuclear charge should be raised by $\sigma_{1s} + \sigma_{2s} = 0.3 + 0.35 = 0.65$. For vacancies in $1s$ $3p$ we have $n = 2$ and $\sigma_{1s} = 1$, the increase in charge should be 1.85. Then come the effects due to the shielding of electrons present in the subshells. It is seen that the s-electrons due to their most spread out wave function have the largest effect because they offer that largest overlap. In a $1s\ 3p$ vacancy the shielding due to $3s$ need be subtracted as $2s$ wave function offers comparatively lesser overlap with $3p$.

Another question that deserves attention is that why the net screenings due to both the states, initial and final have to be added ? This is perhaps because the emission of a line occurs during the time when vacancies exist in both the states : before the emission only the initial state has a vacancy, after the emission only the final state has the vacancy, but during the transition both the states have vacancies. The above attempt is merely a speculation rather than reasoning based on exact quantum mechanical calculations.

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