Investigation of the characteristic spectra as a function of the element's atomic number: L-lines

Objects of the experiment

- Recording of L-lines x-ray fluorescence spectra for several elements.
- Investigation of the structure of the L-series.
- Drawing up of a Moseley's diagram and determination of the atomic screening constant for the electrons of the L-shells.

Principle

When operating the x-ray tube, in addition to the continuous bremsstrahlung, characteristic radiation is also radiated (also see e.g. LD Physics Leaflet P6.3.3.2). In contrast to the bremsstrahlung, the characteristic radiation does not possess a continuous distribution of radiation intensity in the spectrum — its spectrum is composed of sharp lines.

The characteristic radiation is generated when the electrons which are accelerated towards the anode in the x-ray tube knock other electrons out of the inner shells of the atoms making up the anode material. The atom ionised in this way then has a vacancy (electron hole) in a lower shell which previously had been full. These electron holes can be filled with electrons from other, weaker bound shells of the atom: e.g. the *K*-shell can be closed by the transition of an electron from the *L*-shell. Such a transition is connected with the emission of a photon. This radiation has only particular discrete photon energies corresponding to the energy difference beween the levels involved, and it is characteristic for every chemical element.

The designations of the characteristic x-ray lines are a combination of the symbol for the electron shell (*K*, *L*, *M* etc.) and a Greek letter (α, β, γ etc.) or Latin letter. The electron shell being referred to is the one which was ionised before the electron transition. For example the designation *K*α-line describes the transition from the *L*-shell into the *K*-shell, *K*β refers to the transition from the *M*-shell to the *K*-shell. The *L*α-lines , *L*β-lines and *L*γ-lines refer to the transitions from the *M*-shell and the *N*-shell to the *L*-shell.

If viewed more closely, it becomes apparent that the historically developed nomenclature of the x-ray lines is not always logical.

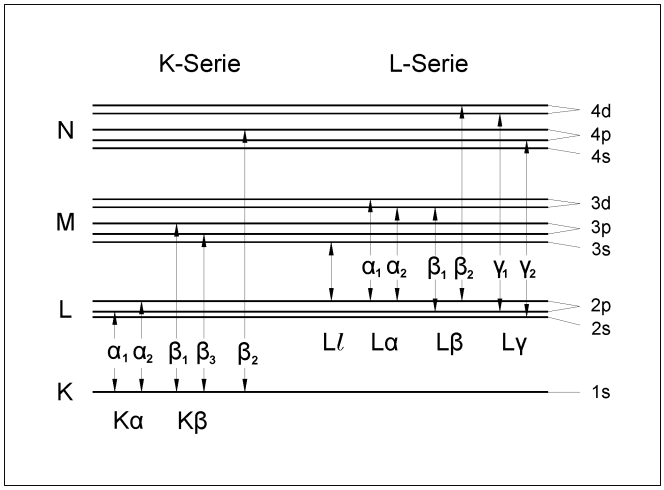

Fig. 1: Simplified terminology diagram of an atom with several characteristic x-ray lines in the K-series and L-series.

The fine structure of the lines, e.g. $L\alpha_1$ and $L\alpha_2$ cannot be resolved in this experiment. Therefore they appear in the spectrum as a single ($L\alpha$) line.

In addition to the *primary* excitation by the electrons in the x-ray tube, the characteristic lines can also be excited through the irradiation of a target with high energy photons. Here the ionisation of the target atom is caused through the absorption of an x-ray photon. This process of *secondary* excitation is also called *x-ray fluorescence*.

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Apparatus

1 set of x-ray apparatus with Mo x-ray tube and goniometer	554 811
or	
1 set of x-ray apparatus with Cu x-ray tube and goniometer	
1 x-ray energy detector	559 938
1 set of targets for L-line fluorescence	554 846
1 CASSY sensor	524 010
1 MCA box	524 058
1 CASSY Lab	524 200
1 HF cable, 1 m	501 02
1 PC with Windows 98/NT or higher	

In order to calculate the energies corresponding to the characteristic lines, the energy levels in the atom (binding energies in the electron shells) have to be known. These can be treated in a similar way to hydrogen by replacing the real charge of the nucleus Z by the effective charge $Z_{eff} = Z - \sigma_n$ with an atomic screening constant σ_n.

The energy of an electron in an inner shell is then approximately represented by a modified Bohr's formula with the principal quantum number n and $Z - \sigma_n$:

$$E_n = -Rhc\,\frac{(Z-\sigma_n)^2}{n^2},$$

with R being the Rydberg constant, $R = m_e e^4 / 8\varepsilon_0^2 h^3 c$. The principal quantum number n refers to the electron shells: n = 1 for the *K*-shell, n = 2 for the *L*-shell, n = 3 for the *M*-shell etc. This formula describes the energy structure of an electron in an inner shell. The atomic screening constant σ_n in general depends on n and Z.

For the frequencies of the characteristic lines $\nu = (E_2 - E_1)/h$ with the transitions $n_2 \to n_1$ ($n_2 > n_1$) the following applies:

$$\nu = cR\left[\frac{(Z-\sigma_{n1})^2}{{n_1}^2} - \frac{(Z-\sigma_{n2})^2}{{n_2}^2}\right].$$

If instead of σ_{n1} and σ_{n2} a single average atomic screening constant $\sigma_{2,1}$ is introduced for the transitions from n_2 to n_1, this formula can be re-written as *Moseley's law*:

$$\sqrt{\frac{\nu}{\nu_R}} = (Z-\sigma_{2,1})\sqrt{\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)}, \qquad \text{(I)}$$

with the Rydberg frequency $\nu_R = cR$. This means that the square root of the frequency of the characteristic lines in one series is a linear function of the atomic number Z. Rewritten to get the energy of the characteristic line, equation (I) becomes:

$$\sqrt{\frac{E}{Ry}} = (Z-\sigma_{2,1})\sqrt{\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)}. \qquad \text{(II)}$$

Here the numerical value for $Ry = Rhc \approx 2.18 \cdot 10^{-18}$ J ~ 13.6 eV.

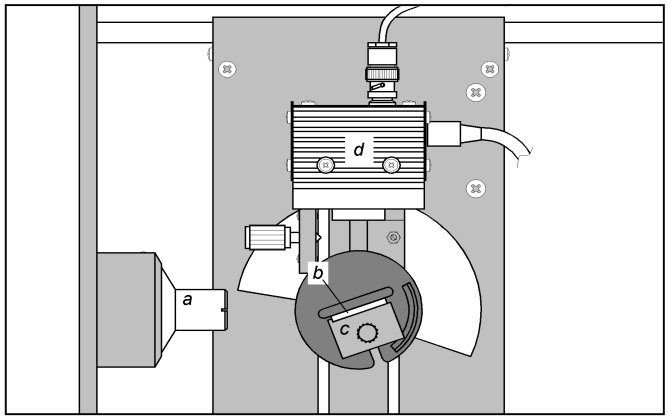

Fig. 2: Experimental setup *a* – collimator, *b* – target, *c* – target table, *d* – detector.

Setup

The experimental set-up is shown in fig. 2.

- Push the connection cable for the table-top device through the empty channel of the x-ray device and connect it to the mini-DIN socket of the x-ray energy detector.
- Secure the sensor holder with the mounted x-ray energy detector in the goniometer sensor arm.
- Connect the signal output of the x-ray energy detector to the BNC socket SIGNAL IN of the x-ray device by means of the BNC cable included.
- Feed enough connection cable through to make complete movement of the sensor arm possible.

This x-ray apparatus fulfils all regulations governing the construction of x-ray apparatus for use in schools and fully protected devices for instructional use, and it is type approved for school use in Germany (NW 807 / 97 Rö).

The built-in protection and screening measures reduce the local dose rate outside the x-ray apparatus to less than 1 µSv/h, a value which is of the same order of magnitude as the natural background radiation.

- Before commissioning the x-ray apparatus, inspect it for damage and check that the high voltage is switched off when the slide doors are opened (see the operating instructions for the x-ray apparatus).
- Protect the x-ray apparatus from access by unauthorised people.

Overheating of the anode in the x-ray tube is to be avoided.

- When switching on the x-ray apparatus, check if the fan in the tube chamber is rotating.

The goniometer is positioned exclusively by means of electric stepper motors.

- Do not block the target arm and the sensor arm on the goniometer and do not use force to move them.

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- Press the SENSOR button and set the sensor angle with the twist adjuster ADJUST manually to 90°.
- Connect sensor CASSY to the computer and connect the MCA box.
- Connect the SIGNAL OUT output in the connection field of the x-ray device to the MCA-box by means of the BNC cable.
- Set the distances between the slit aperture of the collimator and the axis of rotation as well as between the axis of rotation and the window of the x-ray energy detector both to 5 to 6 cm.
- Place the silver (Ag) target from the L-line fluorescence target set onto the target table.
- Press the TARGET button and adjust the target angle manually using the twist button ADJUST to 45°.

Carrying out the experiment

- Connect the table-top device to the mains (after approx. 2 min the LED of the x-ray energy detector will glow green and the device will be ready for use).
- Call CASSY Lab and set the measuring parameters "Multi-channel measurement, 512 channels, negative pulses, amplification = -2.5, measuring duration = 300 s".
- Set the tube high voltage U = 35 kV, emission current I = 1 mA and switch the high voltage on.
- Start the spectrum recording by clicking on  or pressing F9.
- Then record spectra for the other targets in the target set for L-line fluorescence.
- Save the entire measurement under a suitable name.

Example of a measurement

From the example of a measurement (fig. 3a-h), it is apparent that the energy of the characteristic lines and the separation between the α-component and the β-component of the L-spectrum series increase with increasing atomic number.

In the spectra of silver, indium and tin the K-lines and L-lines are simultaneously present. With the heavier elements, other components of the L-series also become apparent.

Note: in addition to the fluorescence lines of the target elements, the scatter of the primary emission (Mo Kα, Kβ) is also apparent in the spectra as well as the fluorescence of the detector housing (Au Lα, Lβ).

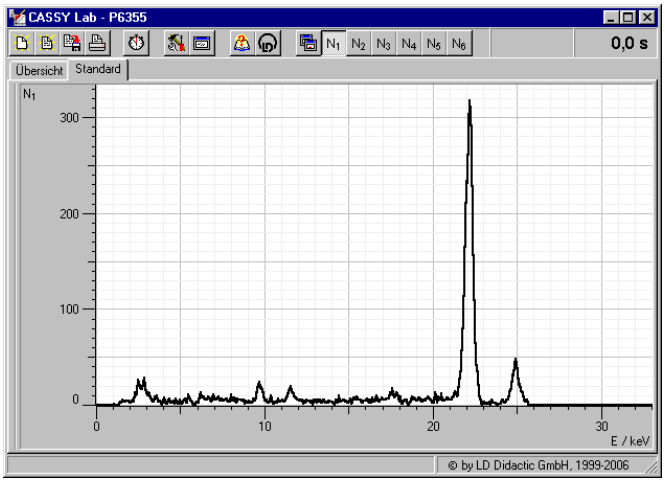

Fig. 3a: X-ray fluorescence spectrum of silver (Ag).

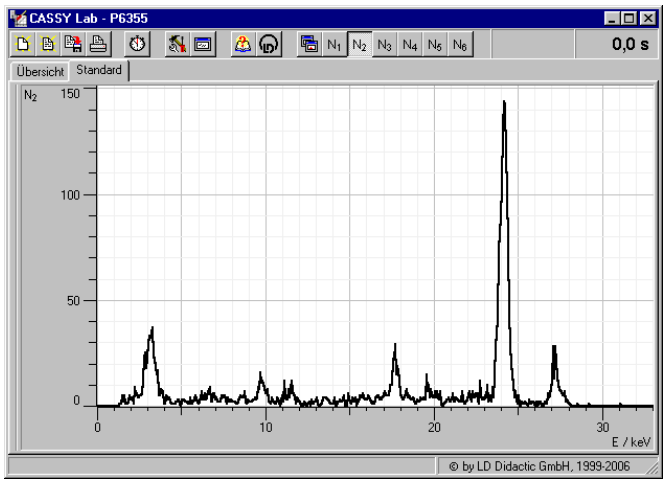

Fig. 3b: X-ray fluorescence spectrum of indium (In).

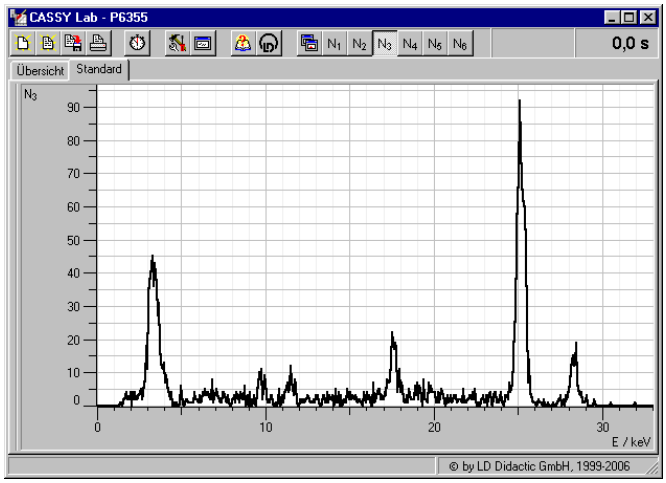

Fig. 3c: X-ray fluorescence spectrum of tin (Sn).

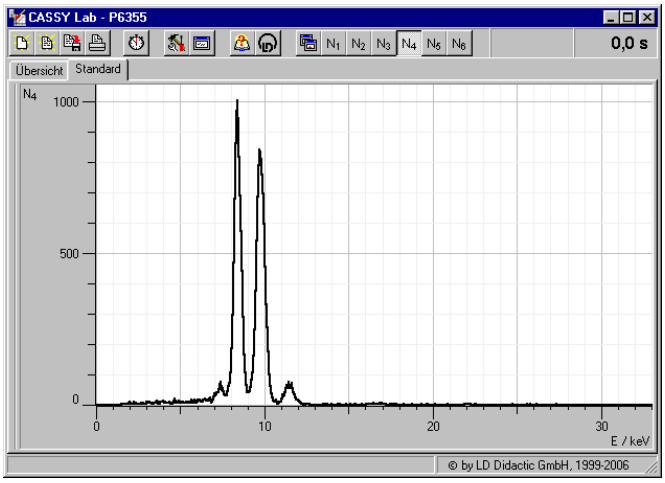

Fig. 3d: X-ray fluorescence spectrum of tungsten (W).

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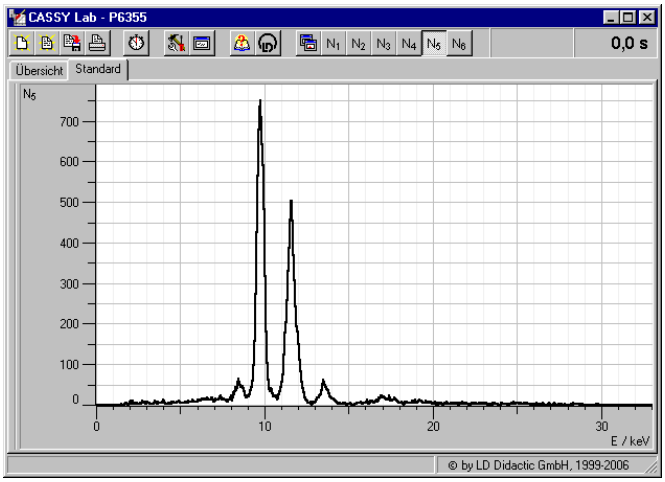

Fig. 3e: X-ray fluorescence spectrum of gold (Au).

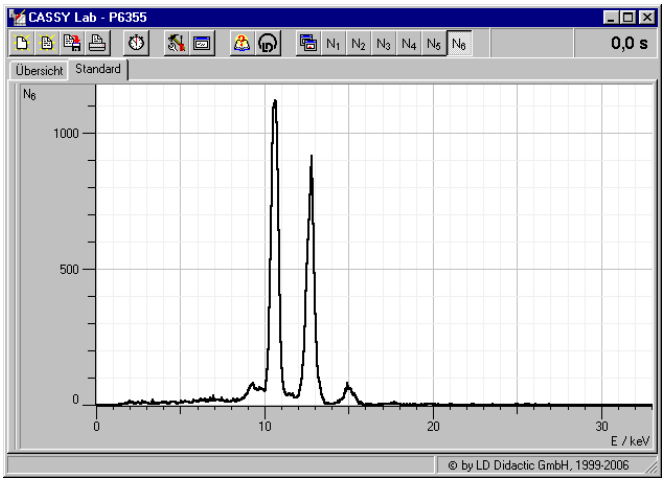

Fig. 3h: X-ray fluorescence spectrum of lead (Pb).

Evaluation and results

a) Identification of the L-series lines

The L-series of the characteristic x-ray radiation includes more lines than the K-series. For the heavier elements, four components of the L-series can be demonstrated with the x-ray energy detector: Ll, Lα, Lβ, and Lγ. Identified gold lines are shown in fig. 4.

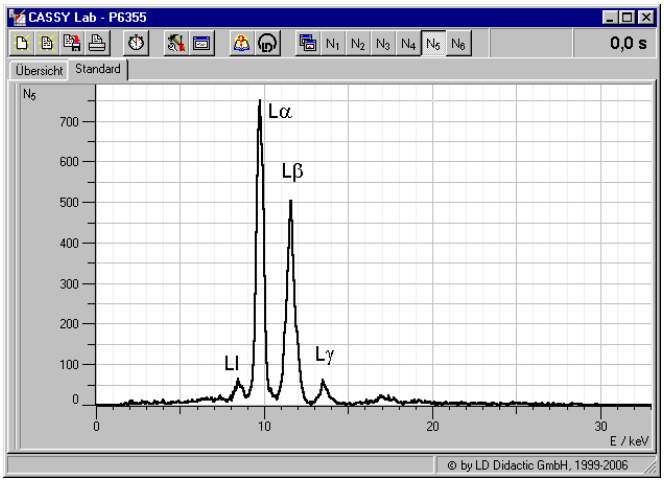

Fig. 4: The L-series of gold with the line designations.

b) Energy calibration of the spectra

The energy calibration of the spectra is made for the Lα-line of tungsten (W) and the Kα-line of silver (Ag).

- Open the "Energy Calibration" dialogue window by pressing Alt+E, select "Global Energy Calibration" and enter the energies for the W Lα-line (8.40 keV) and the Ag Kα-line (22.17 keV).
-
- The spectra of silver and tungsten are to be selected in succession.
- In the popup menu of the diagram window select the menu item "Other evaluations" → "Calculate peak center", select the W Lα-line and enter the result in the "Energy calibration" dialogue window.
- Then determine the center for the Ag Kα-line and enter it.

c) Investigation of the dependency of the energy of the L-lines on atomic number and calculation of the atomic screening constants

For the quantitative analysis the energies of the individual lines are determined:

- Select the energy spectrum.
- In the popup menu of the diagram window select the menu item "Other Evaluations" → "Calculate Peak Center", select the line.
- Read the peak positions found from the status line and enter them into a table (see table 1).

Note: Because for the elements silver, indium and tin the Lα-line and Lβ-line are not resolved, they will be treated in the evaluation as a single line.

- For each line calculate the expression $\sqrt{E/Ry}$ and $\sigma_{2,1}$ using equation (II) and enter them into the table.

Tab. 1 *E*xperimentally determined energies *E* of the K-lines and the atomic screening constants σ_α and σ_β for the corresponding electron transitions.

Element	*Z*	Kα-line			Kβ-line		
		E, keV	$\sqrt{\frac{E}{Ry}}$	σ_α	*E, keV*	$\sqrt{\frac{E}{Ry}}$	σ_β
Ag	47	2.74	14.2	8.9	2.74	14.2	8.9
In	49	3.16	15.2	8.1	3.16	15.2	8.1
Sn	50	3.37	15.7	7.8	3.37	15.7	7.8
W	74	8.40	24.85	7.31	9.76	26.79	2.12
Au	79	9.75	26.77	7.15	11.60	29.20	0.63
Pb	82	10.60	27.92	7.09	12.74	30.61	-0.13

Creation of Moseley's diagram in CASSY Lab:

- Set up a new variable "Atomic number" (as parameter, symbol: Z, from: 0, to: 90, decimal places: 0).
- Set up a new variable "Moseley alpha" (as parameter, symbol: y_&a, from: 0, to: 40, decimal places: 2).
- Set up a new variable "Moseley beta" (as parameter, symbol: y_&b, from: 0, to: 40, decimal places: 2).
- Set up a new diagram called "Moseley" with the atomic number for the x-axis and y_α , y_β for the y-axis.
- Into the table for the "Moseley" diagram enter atomic number and the values of $\sqrt{E/Ry}$ for the α-lines (as y_α) and the β-lines (as y_β) (see fig. 5).
- Select "Moseley" diagram and in the popup menu of the diagram window the menu item "Fit Function" → "Best-fit Straight Line".
- Select the values of y_α in the diagram.
- Also fit a line to the values of y_β.

The result will show an approximately linear dependency of the energies of the L-lines on the atomic number (see fig. 5). The average screening constant for the transitions is the intersection of the fitted line with the x-axis.

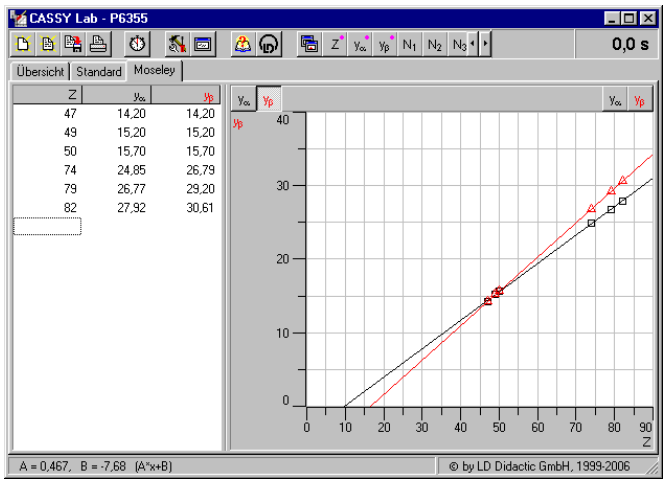

Fig. 5 Dependency of the energies of the L-lines of the atomic number (Moseley's diagram). Shown are the values for $\sqrt{E/Ry}$ for the Lα-lines (y_α, squares) and the Lβ-lines (as y_β, triangles) and the fitted straight line.

Dependence of the screening constants on the atomic number:

- Set up a new variable σ_α (as parameter, name: "screening alpha", symbol: S &s_&a, from: -1 to 10, decimal places: 2).
- Set up a new variable σ_β (as parameter, name: "Screening beta", symbol &s_&b, from: -1 to 10, decimal places: 2).
- Set up a new diagram called "Screening " with the atomic number for the x-axis and σ_α, σ_β for the y-axis.
- Into the tables for the "Screening " diagram enter atomic number and the values of σ_α for the α-lines and of σ_β for the β-lines (see fig. 6).

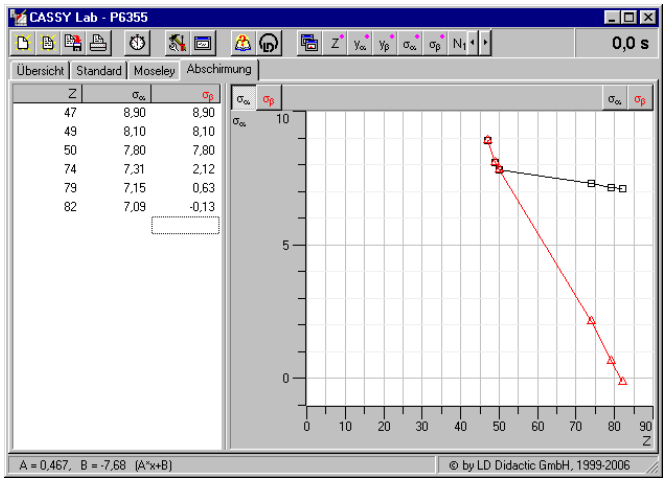

Fig. 6 Effective atomic screening constants for the electron transitions for the L-lines.

The very different dependence of the atomic screening constants for the Lα-line and Lβ-line of the atomic number Z indicates the differences in structure and the sublevels in the *M*-shell and the *L*-shell. It is remarkable that the atomic screening constant for the *L*α-lines has a value of ≈ 7. This means that the screening is provided by the seven electrons remaining in the *L*-shell after ionisation. This again indicates that the *p*-orbitals and *s*-orbitals (*L*-shell or *K*-shell) have such a form that the two electrons in the K-shell are ineffective at screening the *L*α-transition.