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Observation of Hydrogenlike and Heliumlike Krypton Spectra

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Hydrogenlike and heliumlike $n=2 \rightarrow n=1$ lines in Kr have been produced and studied for the first time. Hydrogenlike $Ly\alpha$ lines have been observed and the fine structure interval has been determined. The absolute energy of the $^1P_1$, $^3P_2$, $^3P_1$ lines of heliumlike Kr have been measured and compared to Multiconfigurational Dirac-Fock Calculations.

1. Introduction

The absolute energy of the $Ly\alpha$ lines of some hydrogenlike or heliumlike heavy ions has been measured only very recently (Ar [1], Fe [2], Cl [3]). These measurements have been carried out in view of studying QED effects on deep levels of hydrogenlike ions and relativistic correlation effects or two-body QED effects on heliumlike ions [4]. All these effects since they scale as Z^4 or Z^3 respectively increase very strongly with the atomic numbers. There is then a growing interest in the study of heavier ions. The heaviest one-electron ion for which radiative corrections have been studied so far is Fe. In this paper we report the first observation of the $Ly\alpha$ lines of hydrogenlike and heliumlike Kr ions prepared at the UNILAC heavy ion accelerator of GSI Darmstadt and studied using a previously described technique [2].

2. Experimental Method

The principle of the experiment was to measure the characteristic X-ray lines emitted in flight by foil excited hydrogenlike and heliumlike Kr ions. The UNILAC delivered Kr ions in the charge state 20+ at 18.5 MeV/amu energy. In order to produce and excite the desired one- and two-electron ions, two 200 μg/cm^2 C foils were used. To make absolute energy measurements of the studied transitions, the velocity of the ions must be known with a good precision. This knowledge enabled us to correct the observed lines for the Doppler effect. We used, for this purpose, an 11 m time-of-flight (TOF) that gave a relative precision of $5 \cdot 10^{-4}$ in energy. The energy loss in the foils at these energies is only known by extrapolation of low energy measurements fitted to Betz like formulae [5]. In order to reduce this source of possible uncertainties we chose to strip the beam in the first C foil before the TOF measurement and to bring the most abundant charge state (34+) to the experimental area where the studied states were excited by the second C foil. The charge state distribution at equilibrium thickness, measured by magnetic deflection [6] is given in Table 1.

The principle of the measurement was exactly the same as that previously carried out for Fe [2]. A flat crystal spectrometer, located 3 m apart from the target, detected the $Ly\alpha$ lines emitted by the beam which were directly compared to the Rb $K\alpha$ lines de-

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Table 1. Charge state distribution of 18.6 MeV/amu Kr 34, 35 and 36+ ions through 500 μg/cm² carbon foils [6]

Ion	34+	35+	36+
%	64	15	1

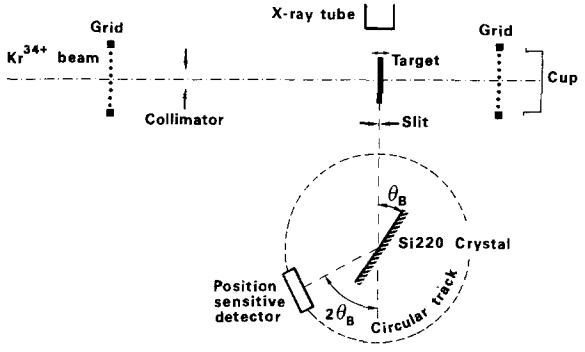

Fig. 1. Schematics of the experimental set-up. Grids are used to control stability and parallelism of the beam

livered by a conventional X-ray tube. The spectrometer was made of a Si 220 crystal working in the second order of reflection and a position sensitive detector of the Backgammon type filled up with a Xe mixture. The crystal was mounted under vacuum on a goniometer, whose precision was of $3 \cdot 10^{-4}$ degree, and moved by a stepping motor. The detector was set on a circular track and its movement controlled with a precision of better than 20 μm ($2\Delta\theta$ movement). The 200 μg/cm² target was moved by a precision translator controlled by a stepping motor in order to adjust the position of the foil in front of the entrance slit of the spectrometer (adjustment of the transmission of the X rays through the slit). The principle of the measurement was to compare the X rays emitted by the Kr ions inside the foil with those emitted by the Rb anode of a conventional X-ray tube located on the other side of the reaction chamber (Fig. 1). The main problem in such an experiment is to control all the parameters for the correction of the very strong Doppler abberations arising at such a high energy. The crystal was first carefully aligned parallel to the ion beam for the definition of a Bragg angle of $\theta = 90°$ for reference. Then, the crystal and the position sensitive detector were adjusted such that the Rb $K\alpha_1$ line was found in the middle of the detector. In a $\Delta\theta - 2\Delta\theta$ movement crystal and detector were rotated to the expected position of the Kr $Ly\alpha$ line emitted at 90° with respect to the beam; thereby, the $Ly\alpha$ line was observed at the same position in the detector as the Rb calibration line. Details of the procedure can be found in [2].

3. The Hydrogenlike Spectrum

The hydrogenlike spectrum we obtained is presented in Fig. 2. Owing to the very low intensity of hydrogenlike excited beam as compared to that of heliumlike, this spectrum was obtained with a widely opened slit in the spectrometer. Therefore it was not possible to make an absolute energy measurement of the lines (such a measurement needs a direct comparison of the Rb $K\alpha$ line and the Kr $Ly\alpha$ line through the same slit). The spectrum presented in Fig. 2 was recorded during a 10 h exposure time at a beam current of about 400 nA. The two $Ly\alpha_1$ and $Ly\alpha_2$ lines were observed over a quite large background, the non uniform structure of which indicates the presence of satellites. Those satellites do not affect appreciably the width of the lines ($\Gamma = 4.5$ eV) that have been found very close to the calculated values and to those of the heliumlike spectrum (The heliumlike spectrum described below does not show appreciable satellite contamination.) The contamination of the observed lines by satellites can obviously provide some errors in the determination of energy of the $Ly\alpha$ lines. The effect of the satellites on the lines has been very carefully studied in the case of Fe by using various foil thicknesses providing a variable amount of satellites [7–8] and has been found to provide, only in the case of hydrogenlike ions, a negligible error. Scaling these results for Kr provides a possible error of less than 0.5 eV, in the position of the two peaks (It must be kept in mind that the observed width, which is very symmetric, is equal to 4.5 eV.)

Although it was not possible to carry out absolute energy measurements of the energies of the transitions in the hydrogenlike ion, our precise knowledge of the energy dispersion of the spectrometer allowed us to determine the energy difference between the two

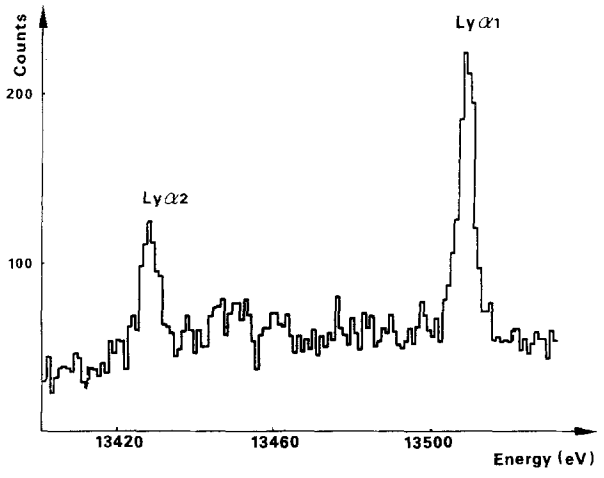

Fig. 2. Hydrogenlike Kr spectrum

Table 2. Comparison of the fine structure splitting measurements with theoretical predictions

Z	Element	Theory	Experiment	Ref.
1	H	10,969.032 MHz	10,969.13 ± 0.1 MHz	[11]
16	S	2.999 eV	2.99 ± 0.02 eV	[12]
17	Cl	3.83 eV	3.84 ± 0.03 eV 3.889 ± 0.03 eV	[3a] [3b]
18	Ar	4.82 eV	5.1 ± 0.3 eV	[1]
22	Ti	10.8 eV	11.05 eV 10.8 eV	13 [14]
26	Fe	21.2 eV	21.1 eV 21.6 eV 21.2 ± 0.2 eV	[15] [16] [10]
36	Kr	79.65 eV[a]	80.8 ± 1.4 eV	This work

[a] For Kr the increase of the fine structure splitting due to the radiative corrections on the two $2p$ levels is equal to 0.155 eV

lines (spin-orbit splitting). The value of the spin-orbit splitting was found to be 80.8 eV ± 1.2. The error in this determination including all the angular calibration errors in the Bragg reflection, detector linearity, and Doppler abberations, does not take into account the error in the Rb $K\alpha_1 - K\alpha_2$ interval measured a long time ago [9]. Including a ± 0.2 eV error for this value the overall error in this measurement is ± 1.4 eV. This fine structure splitting is compared in Table 2 to the theoretical prediction and is found in reasonable agreement with the Dirac equation even though at the upper limit of the error bar.

The theoretical value of fine structure of a hydrogenlike ion is directly given from the Dirac equation. The radiative corrections on the $2p$ levels are very small (Table 2) and are negligible compared to experimental uncertainties. It must be emphasized, however, that the measurement of the fine structure interval for such a heavy ion allows, for the first time, to check the diamagnetic effect on the spin-orbit interaction. When calculated in first order perturbation theory, the spin-orbit splitting is obtained from the classical formulae $W = \boldsymbol{\mu}\mathbf{B}$ and $\Delta H = f(r)\mathbf{L}\cdot\mathbf{S}$. These classical formulae do not include the perturbation (polarization) of the electron orbit by the magnetic field induced by the magnetic moment of the electron orbit (diamagnetic effect), whereas the Dirac equation includes all the terms, the first of them being the diamagnetic ones. The neglect of this "reaction" effect is at the basis of the hypothesis of the magnetostatics. The diamagnetic effect is usually very small but increases strongly with the atomic number of the ion. Up to now, even with the very high accuracy at which the fine structure is measured for hydrogen, the experimental precision has never been large enough to allow the observation of this diamagnetic effect, i.e. no experiment has ever permitted to observe the difference between the magnetostatic perturbation calculation and the full Dirac prediction. For Kr the perturbation calculation provides a value of 75.6 eV while the Dirac equation gives 79.55 eV, the difference between the two numbers (3.95 eV) being much larger than the experimental uncertainties (± 1.4 eV). In Table 2 are presented all the measurements available on this spin-orbit splitting. Among them, only the newly measured spin-orbit splitting of Fe [9] which is now found in good agreement with theory, was sensitive though to a smaller extent to this effect. All the measurements are in good agreement with theory even if some of them are just at the upper limit of the error bar, a fact that cannot be considered as significant.

4. The Heliumlike Spectrum

The heliumlike spectrum observed is presented in Fig. 3. As the intensity for these ions is about ten times larger than for the hydrogenlike ions, the spectrum could be obtained by using the narrow entrance slit of the spectrometer, allowing then an absolute energy measurement. The experiment was carried out in the same procedure as before. The apparent energy of the line was then directly measured with a precision depending only on the statistics and on the precision of the goniometer (1″ of arc). This value was then corrected for the Doppler effect. The correction relied upon the precision of the alignment of the spectrometer which was better than 10^{-2} degree. This leads to an overall estimated error of ± 1.2 eV for the $^1P_1$ line and for values slightly larger for the two other

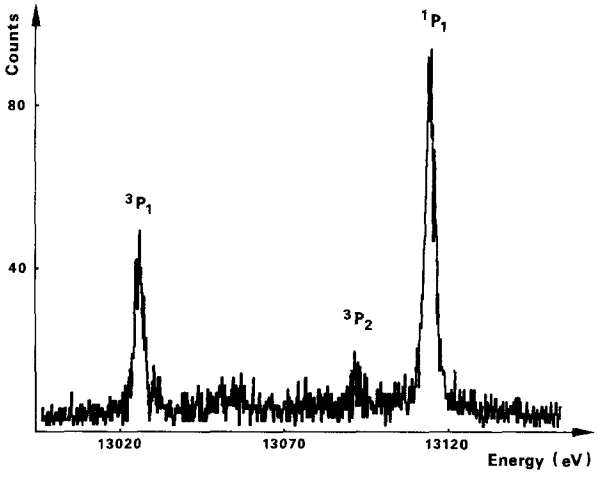

Fig. 3. Heliumlike Kr spectrum

Table 3. Comparison of the experimental values of the energy of heliumlike Kr transitions with theoretical calculations (in eV)

	$^1P_1$	$^3P_1$	$^3P_2$
Experiment	13,113.8±1.2	13,023.8±2.2	13,091.28±1.5
MCDF[a]	13,114.92	13,026.58	13,091.28
1/Z Expansion[b]	13,112.91 [13,113.78]	13,028.31 [13,029.13]	13,091.17 [13,091.97]
RRPA[c]	13,115.25	13,026.89	
RRPA[d]	13,117.22	13,026.5	

[a] This work
[b] Safronova (1980) [17]. Unscreened Lamb shift (calculations corrected for screened Lamb shift from this work are in [17])
[c] Drake [18]. Corrected for screened Lamb shift
[d] Johnson. Private communication

Table 4. Various contributions to the transition energy (in eV)

Contribution (eV)	$^1P_1 \rightarrow {}^1S_0$	$^3P_1 \rightarrow {}^1S_0$	$^3P_2 \rightarrow {}^1S_0$
Dirac-Fock	13.139.97	13,051.88	13,116.88
Breit interaction	−15.97	−16.02	−16.46
Electrostatic correlations	1.10	1.10	1.09
Magnetic correlations	0.44	0.44	0.44
Hydrogenic Lamb shift	−11.49	−11.64	−11.49
Screening of the Lamb shift	0.87	0.82	0.80
Total	13,114.92	13,026.58	13,091.28
Experiment	13,113.8 ±1.2	13,023.8 ±2.2	13,091.2 ±1.5

lines owing to the fact that they are detected far from the calibrating line. The experimental energy values are presented in Table 3. As shown in Fig. 3 the spectrum does not exhibit any measurable contamination by satellites. The lack of far satellites corresponding to n=2 or 3 extra electron clearly shows that no $n \geqq 3$ electron is present in the ions and no lines have to be expected "inside" the considered ones, a fact that is in good agreement with the measured widths of the lines and their perfect symmetries [4]. The experimental values are compared in Table 3 with available theoretical calculations and MCDF ones we performed. Table 4 shows the different contributions in our calculations to the theoretical value of the energy of the considered lines. Table 5 also presents the contributions of the different configurations to the Breit term. Like in the case of heliumlike Fe two main problems have to be solved for such heavy elements (*i*) the magnetic correlation effects which we took as the difference between the values of the Breit term in mono- and multiconfigurational calculation and

Table 5. Contribution of various configurations to the value of the Breit term (in eV)

Configuration	Total energy[a]	ΔE[b]	Breit term	Weight[c]
$1s^2$	35,270.75	0	−16.81	0.99998
$+2s^2$	35,271.14	0.39	−16.70	0.730 (−5)
$+2p^2$	35,271.76	1.01	−16.47	0.115 (−6)
$+3s^2$	35,271.78	1.03	−16.45	0.164 (−6)
$+3p^2$	35,271.84	1.09	−16.41	0.407 (−6)
$+3d^2$	35,271.91	1.16	−16.37	0.581 (−6)

[a] Without Breit and relative corrections
[b] Contribution of the correlation energy due to electrostatic interactions
[c] Coefficient squares of the configuration state function as determined by the self-consistent Dirac-Fock process. Numbers in parentheses are powers of ten

(*ii*) the two-body QED effects (screening of the Lamb shift).

(*i*) The mean value of the Breit interaction (magnetic and retardation effects) between the two electrons in the ground state, found equal to 16.81 eV in single configurational calculations, is equal to 16.37 eV in multiconfigurational ones. It gives a value of 0.44 eV for magnetic correlations to be compared to 1.16 eV for electrostatic ones. Calculations made for different values of Z show that these magnetic correlations scale approximately as Z^2 (as expected from the double series expansion of Layzer and Bahcall [20] while the electrostatic ones are approximately constant (for high Z again as expected from the Z expansion of the non relativistic total energy).

(*ii*) The second problem is the effect of the screening of the Lamb shift. When taking account of the effective nuclear charge for each orbital, computed by solving $\langle r_{\text{MCDF}} \rangle = \langle r_{\text{hydrogenic}} (Z_{\text{eff}}) \rangle$, one finds −10.62 eV to be compared to −11,49 eV (for $2\,^1P_1 \rightarrow 1\,^1S_0$ transition) of the hydrogenic calculation (in both cases the self energy values are obtained by interpolation between Mohr values [21] as described in [4]. This effect is then the half of the total correlations in the $1s^2$ state.

The sum of these two effects is then close to the experimental uncertainty and is not out of the range of further experimental improvements.

In conclusion the agreement between experiment and theoretical predictions is already very satisfactory (Table 3) except in the case of the $^3P_1$ level the energy of which is found slightly outside the error bar.

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