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Transitions Within the $n = 4$ Complex of Kr VII Obtained from a Theta-Pinch Light Source

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Abstract

The spectrum of six times ionized krypton (Kr VII) has been observed in the 430–1000 Å wavelength range and 23 lines have been identified as transitions between levels of the $4s^2$, $4s4d$, $4p^2$ and $4s4p$ configurations. For 13 of the lines the classification is new. Revised values are proposed for three levels while for the rest the uncertainty in the existing level values has been considerably decreased.

The results are supported by isoelectronic comparisons along the Zn I isoelectronic sequence. The configurations are interpreted by fitting the theoretical energy expressions to the observed energy levels using least-squares techniques. The parameter values are compared with results from Hartree-Fock calculations.

1. Introduction

The Kr^{6+} ion belongs to the Zn I isoelectronic sequence. The knowledge of the spectra in this sequence with the exception of the Zn I spectrum was for a long time limited [1]. A small number of levels were reported for Ga II–Br VI [1], but for Kr VII and more highly ionized ions, no information was available. For Zn I the analysis presented in Atomic Energy Levels [1] has been extended [2–4], and a few levels of Ga II [5] were added by Denne et al. Recently Isberg and Litzén revised and extended the analysis of Ga II [6]. The analyses of Se V and Br VI have also been extended [7, 8]. For more highly ionized ions the $4s$–$4p$ resonance transition of Rb VIII–Mo XIII and Ru XV–Dy XXXVII was observed by Reader and Acquista [9, 10]. Litzén and Ando reported the $4s$–$4p$ transitions including intercombination lines in Zr XI, Nb XII and Mo XIII [11]. Observations of the Kr VII spectrum were reported by Fawcett et al. using a zeta-pinch [12]. Several reports on observations of Kr VII spectra using the beam-foil technique [13–16] have appeared. The Zn I isoelectronic sequence has been studied theoretically in a number of papers [17–20].

The present work concerns the study of the $4s^2$, $4s4d$, $4p^2$ and $4s4p$ configurations in Kr VII.

The revival of the interest in data on the Zn I isoelectronic sequence is due to observations of impurity-lines from highly ionized heavy ions with few valence electrons in high temperature plasmas [21, 22]. Such lines have been used for diagnostic purposes. The resonance transition $4s^2\ {}^1S_0$–$4s4p\ {}^1P_1$ has been observed for a large range of Z values in the Zn I isoelectronic sequence [9, 23].

2. Experimental arrangements

The light source used in the present work is a theta-pinch discharge built at Lund Institute of Technology [24].

The spectra were recorded using a 3 m normal-incidence spectrograph equipped with a 1200 lines/mm grating blazed for 1380 Å. The plate factor in the first diffraction order is 2.77 Å mm^{-1}.

To distinguish between different stages of ionization, a number of experimental parameters, i.e., gas pressure, discharge voltage and number of discharges, were varied. A well developed Kr VII spectrum was obtained with the following parameters: 4 mTorr, 13 kV and 800 discharges.

The spectra were exposed on Kodak SWR plates and lines from C III, N III, O III, Kr II and Kr III were used as internal standards. The plates were measured with a semi-automatic comparator with a photoelectric setting device [25]. For sharp lines the settings are reproducible to within $\pm 0.5\,\mu$m. Third order interpolation formulas, together with correction curves, were employed to reduce the comparator settings to wavelength values. The accuracy of the wavelength values is estimated to be ± 0.01 Å.

3. Analysis

The Kr VII lines observed in the present work are given in Table I, 13 of them being without previous classification. The intensity figures given in the table are based on visual estimates.

The energy levels derived from the observed lines are given in Table II, and the general structure of the term system is shown in Fig. 1. When establishing the energy levels, we were guided by isoelectronic comparisons taking into account Zn I [1], Ga II [6], Ge III [1], As IV [1], Se V [7] and Br VI [7, 8].

When performing the analysis we also used theoretical predictions of the structures of the configurations. The predictions were obtained by diagonalizing the energy matrices with appropriately scaled Hartree–Fock (HF) values for the energy parameters. For this purpose the computer code developed by Cowan [26] was used. A comparison with the level system given by Pinnington et al. [16] shows that eight of their levels values have been confirmed, although the accuracy has been considerably improved. However, for three levels we propose new identifications as discussed below.

For the level $4s4p\ {}^3P_0$ we propose the new value 117 389 cm^{-1}. The level is established from a line at 617.18 Å, classified as the $4s4p\ {}^3P_0$–$4p^2\ {}^3P_1$ transition. This position is in reasonable agreement with the value predicted by Curtis [20].

For the level $4s4d\ {}^3D_1$ we propose a new value at 349 973 cm^{-1}. The level is determined by a line at 558.22 Å

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Table I. *Identified lines of Kr VII*

Intensity	λ(Å)	σ(cm^{-1}) Obs.	Calc.	Combination
15	434.140[a]	230 340.4	22.0	$4s4p\ ^3P_1$–$4s4d\ ^3D_2$
8	435.018	229 875.5	8.3	$^3P_1$– $^3D_1$
20	445.309	224 563.2	.2	$^3P_2$– $^3D_3$
8	446.700	223 863.9	.8	$^3P_2$– $^3D_2$
3	447.606	223 410.8	20.1	$^3P_2$– $^3D_1$
25	479.264	208 653.3	.3	$^1P_1$– $^1D_2$
4	556.855	179 580.0	1.8	$^1P_1$– $^3D_2$
4	558.221	179 140.5	38.1	$^1P_1$– $^3D_1$
15	585.361	170 834.8	5.0	$4s^2\ ^1S_0$–$4s4p\ ^1P_1$
30	594.899	168 095.8	.4	$4s4p\ ^3P_1$– $4p^2\ ^3P_2$
30	617.189	162 024.9	.9	$^3P_0$– $^3P_1$
40	618.664	161 638.6	7.2	$^3P_2$– $^3P_2$
4	626.486	159 620.5	.0	$^3P_1$– $^1D_2$
30	627.668	159 319.9	.7	$^3P_1$– $^3P_1$
30	645.847	154 835.4	6.9	$^3P_1$– $^3P_0$
5	652.905	153 161.6	.8	$^3P_2$– $^1D_2$
50	654.189	152 861.0	.5	$^3P_2$– $^3P_1$
9	832.682	120 093.9	4.8	$4s^2\ ^1S_0$–$4s4p\ ^3P_1$
5	852.120	117 354.4	5.2	$4s4p\ ^1P_1$– $4p^2\ ^3P_2$
60	918.446	108 879.6	.8	$^1P_1$– $^1D_2$
5	920.983	108 579.6	.5	$^1P_1$– $^3P_1$
5	960.638	104 097.5	6.7	$^1P_1$– $^3P_0$

[a] Asymmetric line.

classified as the $4s4p\ ^1P_1$–$4s4d\ ^3D_1$ transition. This identification is confirmed by the lines at 435.01 Å and 447.60 Å corresponding to the $4s4p\ ^3P_1$–$4s4d\ ^3D_1$ and $4s4p\ ^3P_2$–$4s4d\ ^3D_1$ transitions. This new level value is in agreement with the theoretically predicted value by Ivanova et al. [19].

For the level $4p^2\ ^1D_2$ we propose the value 279 714 cm^{-1}, determined by a line at 918.45 Å and classified as the $4s4p\ ^1P_1$–$4p^2\ ^1D_2$ transition. The identification is confirmed by a line at 626.48 Å classified as $4s4p\ ^3P_1$–$4p^2\ ^1D_2$ and a line at 652.90 Å classified as $4s4p\ ^3P_2$–$4p^2\ ^1D_2$. This new level value fits well with the graphic prediction that can be made from the work by Litzén and Ando [11]. The calculated eigenvector composition shows that this level is strongly mixed with the level $4p^2\ ^3P_2$. In the work by Ivanova et al. [19] the two designations are interchanged but we prefer to maintain the old designation.

Table II. *Energy levels of Kr VII*

Designation	Energy (cm^{-1})	Obs.–Calc. (cm^{-1})	Percentage[a] composition
$4s^2\ ^1S_0$	0.0		98
$4s4p\ ^3P_0$	117 389.6	9	100
$^3P_1$	120 094.8	13	100
$^3P_2$	126 553.0	3	100
$^1P_1$	170 835.0	0	100
$4p^2\ ^3P_0$	274 931.7	0	98
$^3P_1$	279 414.5	0	100
$^3P_2$	288 190.2	1	$72p^2\ ^3P + 22p^2\ ^1D + 4sd\ ^1D$
$^1D_2$	279 714.8	1	$62p^2\ ^1D + 27p^2\ ^3P + 11sd\ ^1D$
$4s4d\ ^3D_1$	349 973.1	2	100
$^3D_2$	350 416.8	4	100
$^3D_3$	351 116.2	1	100
$^1D_2$	379 488.3[b]	0	$85sd\ ^1D + 15p^2\ ^1D$

[a] Percentages lower than 4% are omitted. The average *LS* purities of the $4s^2$, $4s4d$ and $4p^2$ configurations are 91% and for $4s4p$ 90%.

[b] This level was determined by one line only.

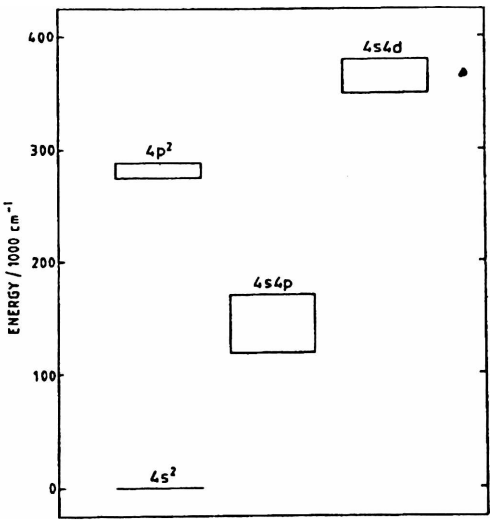

Fig. 1. The gross structure of the lower part of the Kr VIII energy level system.

Table III. *Energy parameters for the 4s4p configuration of Kr VII*

Parameter	HF value (cm^{-1})	Fitted value[a] (cm^{-1})	Fit/HF
E_{av}	117 277	135 244	1.153
$G^1(4s, 4p)$	93 240	70 442	0.755
ξ_{4p}	5 256	6 105	1.161

[a] The rms deviation of the fit is 17 cm^{-1} for 4 observed levels.

Table IV. *Energy parameters for the $4s^2$, $4s4d$, $4p^2$, $4s5s$ and $4d^2$ configurations of Kr VII*

Configuration	Parameter	HF value (cm^{-1})	Fitted value[a] (cm^{-1})	Fit/HF
$4s^2$	E_{av}	0	9 269	
$4s4d$	E_{av}	330 775	354 121	1.071
	$G^2(4s, 4d)$	54 420	34 635	0.636
	ξ_{4d}	406	458	1.128
$4p^2$	E_{av}	260 760	292 271	1.121
	$F^2(4p, 4p)$	70 181	68 692	0.979
	ξ_{4p}	5 241	6 138	1.171
$4s5s$	E_{av}	419 161	419 161(fix)	1.000
	$G^0(4s, 5s)$	3 203	3 203(fix)	1.000
$4d^2$	E_{av}	677 283	677 283(fix)	1.000
	$F^2(4d, 4d)$	57 766	57 766(fix)	1.000
	$F^4(4d, 4d)$	38 999	38 999(fix)	1.000
	ξ_{4d}	425	425(fix)	1.000
Configuration interaction integrals				
$4s^2$–$4p^2$	$R^1(4s4s, 4p4p)$	93 147	93 147(fix)	1.000
$4s^2$–$4d^2$	$R^2(4s4s, 4d4d)$	56 228	56 228(fix)	1.000
$4s4d$–$4p^2$	$R^1(4s4d, 4p4p)$	81 966	73 052	0.891
$4s4d$–$4d^2$	$R^2(4s4d, 4d4d)$	54 838	54 838(fix)	1.000
$4p^2$–$4s5s$	$R^1(4p4p, 4s5s)$	−5 944	−5 944(fix)	1.000
$4p^2$–$4d^2$	$R^1(4p4p, 4d4d)$	76 105	76 105(fix)	1.000
	$R^3(4p4p, 4d4d)$	47 659	47 659(fix)	1.000
$4s5s$–$4d^2$	$R^2(4s5s, 4d4d)$	−12 341	−12 341(fix)	1.000

[a] The rms deviation of the fit is 5 cm^{-1} for 9 observed levels.

This is in accordance with our theoretical prediction and with the graphic extrapolation along the isoelectronic sequence shown in the work of Litzén and Ando [11].

4. Theoretical interpretation

The level structure was theoretically interpreted by a least-squares fit of the energy parameters to the experimental level values. The computer code by Cowan [26] was used (Tables III and IV). In the calculation for the even parity configurations, i.e., $4s^2$, $4s4d$ and $4p^2$, configuration interaction was included. The experimentally unknown $4s5s$ and $4d^2$ were also included in the theoretical calculation. The configuration interaction parameters were kept fixed at their Hartree–Fock (HF) values. However, due to the strong interaction between the terms $4p^2\ ^1D$ and $4s4d\ ^1D$ [17] the configuration interaction parameter $R^1(4s4d, 4p4p)$ was free to vary. This reduced the mean error of the least-squares fit from 56 cm^{-1} to 5 cm^{-1}.

The odd parity $4s4p$ configuration was interpreted without inclusion of configuration interactions, the reason being that the only experimentally known levels belong to this configuration.

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References

1. Moore, C. E., Atomic Energy Levels, Vol. II, National Bureau of Standards, U.S.A. (1971).
2. Johansson, I. and Contreras, R., Arkiv för Fysik **37**, 513 (1968).
3. Brown, C. M., Tilford, S. G. and Ginter, M. L., J. Opt. Soc. Am. **65**, 1404 (1975).
4. Martin, W. C. and Kaufman, V., J. Opt. Soc. Am. **60**, 1096 (1979).
5. Denne, B., Litzén, U. and Curtis, L. J., Phys. Lett. **71A**, 35 (1979).
6. Isberg, B. and Litzén, U., Physica Scripta **31**, 533 (1985).
7. van Kleef, T. A. M. (private communication).
8. Curtis, L. J., Martinson, I., Leavitt, J. A., Dietrich, D. D., Bashkin, S. and Denne, B., Phys. Lett. **105A**, 212 (1984).
9. Reader, J. and Acquista, N., Phys. Rev. Lett. **39**, 184 (1977).
10. Acquista, N. and Reader, J., J. Opt. Soc. Am. **B1**, 649 (1984).
11. Litzén, U. and Ando, K., Phys. Lett. **10A**, 411 (1984).
12. Fawcett, B. C., Jones, B. B. and Wilson, R., Proc. Phys. Soc. London **78**, 1223 (1961).
13. Druetta, M. and Buchet, J. P., J. Opt. Soc. Am. **66**, 433 (1976).
14. Irwin, D. J. G., Kernahan, J. A., Pinnington, E. H. and Livingston, A. E., J. Opt. Soc. Am. **66**, 1396 (1976).
15. Livingston, A. E., J. Phys. **B9**, L215 (1976).
16. Pinnington, E. H., Ansbacher, W. and Kernahan, J. A., J. Opt. Soc. Am. **B1**, 30 (1984).
17. Froese Fischer, C. and Hansen, J. E., Phys. Rev. **A19**, 1819 (1979).
18. Victor, G. A. and Taylor, W. R., Atomic Data and Nuclear Data Tables **28**, 107 (1983).
19. Ivanova, E. P., Ivanov, L. N., Gurchumelya, A. D., Tsirekidze, M. A. and Tsirekidze, T. A., J. Phys. **B18**, 1467 (1985).
20. Curtis, L. J., J. Opt. Soc. Am. **B2**, 407 (1985).
21. Hinnov, E., Phys. Rev. **A14**, 1533 (1976).
22. Finkenthal, M. et al., Phys. Lett. **82A**, 123 (1981).
23. Reader, J. and Luther, G., Phys. Rev. Lett. **45**, 609 (1980).
24. Pettersson, S.-G., Physica Scripta **26**, 296 (1982).
25. Gunnvald, P., Arkiv för Fysik **22**, 333 (1962).
26. Cowan, R. D., The Theory of Atomic Structure and Spectra, Univ. of California Press, Berkeley, U.S.A. (1981).