Article

New Transition and Energy Levels of Three-Times Ionized Krypton (Kr IV)

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Abstract: A capillary pulsed-discharge and a theta-pinch were used to record Kr spectra in the region of 330–4800 Å. A set of 168 transitions of these spectra were classified for the first time. We extended the analysis to twenty-five new energy levels belonging to $3s^23p^24d$, $3s^23p^25d$ even configurations. We calculated weighted transition probabilities (gA) for all of the experimentally observed lines and lifetimes for new energy levels using a relativistic Hartree–Fock method, including core-polarization effects.

Keywords: atomic spectra; energy levels; pulsed-discharge; relativistic Hartree–Fock calculations

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1. Introduction

Krypton that has been three-times ionized, Kr IV, belongs to the arsenic isoelectronic sequence. The most recent and complete compilation of the observed energy levels and transitions of the Kr IV ion was reported by Saloman [1]; that work used the extended analysis of our group (Reyna Almandos et al. [2]) for all but two Kr IV levels, 208,920 and 231,940 cm^{-1} , which they took from Sugar and Musgrove [3]. The observed spectral lines of Kr IV were published by Saloman [1] from six sources: Boyce [4], Irwin et al. [5], Livingston [6], Fawcett and Bromage [7], Persson and Pettersson [8], and Bredice et al. [9]. The spectra of ions along the sequence of As I have been studied over many years [2] (references cited therein). These data and other recently published data on the arsenic isoelectronic sequence, for example, Rb V [10] and Y VII [11], were reported by NIST [12]. Reliable values of oscillator strengths, transition probabilities, and radiative lifetimes of energy levels are essential for the study of the ionized noble gases in Kr IV [9]; also, for astrophysical applications, for example, calculating Kr IV–VII oscillator strengths to consider radiative and collisional bound–bound transitions in detail in the non-LTE stellar-atmosphere models for the analysis of Kr lines that are exhibited in high resolution and high S/N ultraviolet (UV) observations of the hot white dwarf RE0503289 [13]. Recently energies and transition parameters have been reported for triply ionized Kr IV, Xe IV, and Rn IV using the general-purpose relativistic atomic structure package based on a fully relativistic multiconfiguration Dirac–Fock method [14]. In this article, we present an extension of the analysis of Kr IV from reference [2], including five energy levels of the configuration $3s^23p^24d$ and twenty levels of the $3s^23p^25d$ configuration. We interpreted this study using Hartree–Fock relativistic (HFR) calculations and parametric fits. We used the Cowan package [15] considering core polarization (CP) effects [16], which is the distortion of the internal cloud by the electric field of the outer electron orbital. For these energy levels, lifetimes were calculated using electron correlation effects. A set of 168 spectral lines of the Kr IV spectrum were classified for the first time; weighted transition probabilities (gA) were also reported for these transitions considering the CP effects.

2. Experiment

Krypton spectra covering the region from 330 to 4800 Å obtained from two different light sources (a capillary-pulsed discharge and a theta-pinch) were used. The discharge tube was built at Centro de Investigaciones Opticas (CIOP) in La Plata to study highly ionized gases [17], and the theta-pinch, used several years ago by A.G.T. and J.R.A. at the Lund Institute of Technology, Sweden, is described in Ref. [18]. Other experimental devices are detailed in reference [19]. A 3-m normal incidence vacuum spectrograph with a concave diffraction grating of 1200 lines/mm and a plate factor of 2.77 Å/mm in the first order was used in both experiments below 2000 Å. C, N, O, and available lines of krypton were recorded as internal standard lines. A wavelength range above 2000 Å was recorded in La Plata on a 3.4-m Ebert plane-grating spectrograph, with a plate factor of 5 Å/mm in the first diffraction order. The lines observed in this interval were measured by polynomial interpolation using reference lines from a thorium ²³²Th lamp, whose wavelengths were determined interferometrically [20]. The uncertainty in the wavelength values for lines that are not classified as *w,d*, or *ul* in Table 1 is ±0.01 Å in the measurements from Lund and ±0.01 Å and ±0.02 Å in the measurements from La Plata for the visible and the vacuum ultraviolet (VUV) regions, respectively. The intensity figures are visual estimates of photographic density and are only on a uniform scale within the limited wavelength ranges. To distinguish among different stages of ionization, we studied the behavior of the spectral line intensity as a function of pressure and discharge voltage. We used the LOPT [21] program to recalculate the energy levels from the observed wavelengths. In this adjustment, we considered the previously known lines [12] and included the new ones. The conversion between the air and vacuum wavelength used as the refraction index of the air was derived from the five-parameter formula given by E.R. Peck and K. Reeder [22].

Table 1. New classified lines of Kr IV.

Int.	λ_{obs} Vac(Å)	λ_{Ritz} (Å)	$\lambda_{obs}-\lambda_{Ritz}$ (Å)	σ_{obs} cm^{-1}	Lower Level			Upper Level			gA	gA(CP)
					Conf.	Term	<i>J</i>	Conf.	Term	<i>J</i>	s^{-1}	s^{-1}
3	333.33	333.306	0.023	300,003	4s ² 4p ³	4S	3/2	4s ² 4p ² (³ P)5d	2P	1/2	3.24 × 10 ⁸	3.21 × 10 ⁸
1	333.52	333.542	−0.022	299,832	4s ² 4p ³	4S	3/2	4s ² 4p ² (³ P)5d	4P	1/2	7.53 × 10 ⁹	4.49 × 10 ⁹
1	337.00	337.024	−0.025	296,736	4s ² 4p ³	4S	3/2	4s ² 4p ² (³ P)5d	4D	3/2	3.11 × 10 ⁹	2.21 × 10 ⁹
1	338.21	338.214	0.000	295,674	4s ² 4p ³	2D	3/2	4s ² 4p ² (¹ D)5d	2P	1/2	2.63 × 10 ⁹	1.56 × 10 ⁹
1	338.21	338.223	−0.010	295,674	4s ² 4p ³	2D	5/2	4s ² 4p ² (¹ D)5d	2P	3/2	8.16 × 10 ⁸	8.64 × 10 ⁸ *
1	338.91	338.901	0.009	295,064	4s ² 4p ³	4S	3/2	4s ² 4p ² (³ P)5d	4P	5/2	1.38 × 10 ¹⁰	9.02 × 10 ⁹
1	339.52	339.542	−0.020	294,533	4s ² 4p ³	2D	3/2	4s ² 4p ² (¹ D)5d	2F	5/2	8.31 × 10 ⁹	5.99 × 10 ⁹
1	339.52	339.524	0.000	294,533	4s ² 4p ³	2D	5/2	4s ² 4p ² (¹ D)5d	2D	5/2	4.71 × 10 ⁹	2.37 × 10 ⁹ *
2	341.44	341.470	−0.030	292,877	4s ² 4p ³	2D	5/2	4s ² 4p ² (¹ D)5d	2F	5/2	1.43 × 10 ¹⁰	1.08 × 10 ¹⁰
1	343.26	343.282	−0.023	291,324	4s ² 4p ³	2D	5/2	4s ² 4p ² (¹ D)5d	2F	7/2	1.43 × 10 ¹⁰	9.50 × 10 ⁹
1	350.88	350.860	0.020	284,998	4s ² 4p ³	2D	5/2	4s ² 4p ² (³ P)5d	2D	3/2	1.30 × 10 ⁹	1.11 × 10 ⁹
1	351.09	351.116	−0.027	284,827	4s ² 4p ³	2D	5/2	4s ² 4p ² (³ P)5d	2D	5/2	7.36 × 10 ⁹	4.28 × 10 ⁹
1	355.88	355.925	−0.045	280,994	4s ² 4p ³	2P	3/2	4s ² 4p ² (¹ D)5d	2P	3/2	6.25 × 10 ⁹	7.53 × 10 ⁹
1	357.54	357.555	−0.015	279,689	4s ² 4p ³	2D	3/2	4s ² 4p ² (³ P)5d	4D	3/2	3.11 × 10 ⁹	2.06 × 10 ⁹
1	359.53	359.523	0.007	278,141	4s ² 4p ³	2P	3/2	4s ² 4p ² (¹ D)5d	2F	5/2	2.99 × 10 ⁸	2.79 × 10 ⁷ *
3	359.65	359.668	−0.018	278,048	4s ² 4p ³	2D	3/2	4s ² 4p ² (³ P)5d	4P	5/2	2.50 × 10 ⁸	1.69 × 10 ⁸ *
5	364.15	364.156	−0.007	274,612	4s ² 4p ³	2D	3/2	4s ² 4p ² (³ P)5d	4F	5/2	1.51 × 10 ⁹	9.84 × 10 ⁸

Table 1. Cont.

1	366.37	366.375	−0.006	272,948	4s ² 4p ³	² D	5/2	−	4s ² 4p ² (³ P)5d	⁴ F	5/2	1.09 × 10 ⁸	7.71 × 10 ⁷
1	366.74	366.758	−0.019	272,673	4s ² 4p ³	² P	1/2	−	4s ² 4p ² (³ P)5d	² D	3/2	1.08 × 10 ¹⁰	8.05 × 10 ⁹
1	369.93	369.947	−0.017	270,321	4s ² 4p ³	² P	3/2	−	4s ² 4p ² (³ P)5d	² D	3/2	3.50 × 10 ⁹	2.08 × 10 ⁹
11	370.22	370.232	−0.012	270,110	4s ² 4p ³	² P	3/2	−	4s ² 4p ² (³ P)5d	² D	5/2	7.95 × 10 ⁹	5.37 × 10 ⁹
1	372.09	372.083	0.007	268,752	4s ² 4p ³	² P	1/2	−	4s ² 4p ² (³ P)5d	⁴ P	1/2	4.13 × 10 ⁸	3.95 × 10 ⁸
1	379.78	379.782	−0.002	263,310	4s ² 4p ³	² P	3/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	7.38 × 10 ⁸	5.14 × 10 ⁸ *
2	480.62	480.656	−0.036	208,065	4s ² 4p ³	² D	3/2	−	4s ² 4p ² (¹ D)4d	² S	1/2	5.29 × 10 ⁹	5.66 × 10 ⁹
3	484.77	484.755	0.015	206,283	4s ² 4p ³	² D	3/2	−	4s ² 4p ² (³ P)4d	² P	1/2	2.21 × 10 ⁹	1.35 × 10 ⁹
5	494.15	494.143	0.007	202,368	4s ² 4p ³	⁴ S	3/2	−	4s ² 4p ² (³ P)4d	⁴ P	3/2	1.46 × 10 ¹¹	1.32 × 10 ¹¹
8	515.35	515.382	−0.032	194,043	4s ² 4p ³	² P	1/2	−	4s ² 4p ² (¹ D)4d	² S	1/2	6.27 × 10 ⁸	5.79 × 10 ⁷
3	520.10	520.097	0.003	192,271	4s ² 4p ³	² P	1/2	−	4s ² 4p ² (³ P)4d	² P	1/2	5.91 × 10 ¹⁰	5.67 × 10 ¹⁰
7	521.70	521.700	0.000	191,681	4s ² 4p ³	² P	3/2	−	4s ² 4p ² (¹ D)4d	² S	1/2	5.82 × 10 ¹⁰	5.35 × 10 ¹⁰
9	544.44	544.453	−0.013	183,675	4s ² 4p ³	² D	5/2	−	4s ² 4p ² (³ P)4d	⁴ P	3/2	1.30 × 10 ⁹	1.28 × 10 ⁹
7	557.75	557.757	−0.010	179,292	4s ² 4p ³	² D	5/2	−	4s ² 4p ² (¹ D)4d	² G	7/2	1.85 × 10 ⁹	1.74 × 10 ⁹
3	591.83	591.836	−0.010	168,967	4s ² 4p ³	² P	3/2	−	4s ² 4p ² (³ P)4d	⁴ P	3/2	3.46 × 10 ⁸	2.84 × 10 ⁸ *
1d	1140.74	1140.768	−0.028	87,662	4s ² 4p ² (³ P)5p	² D	3/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	1.37 × 10 ⁸	1.41 × 10 ⁸
7	1148.17	1148.196	−0.026	87,095	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	2.79 × 10 ⁶	2.67 × 10 ⁶ *
10	1177.21	1177.216	−0.006	84,947	4s ² 4p ² (³ P)5p	⁴ S	3/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	1.62 × 10 ⁷	1.97 × 10 ⁷ *
9	1214.30	1214.288	0.012	82,352	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	9.48 × 10 ⁶	8.93 × 10 ⁶ *
9	1228.72	1228.723	−0.003	81,385	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	5.88 × 10 ⁶	1.34 × 10 ⁷ *
10	1237.02	1237.030	−0.010	80,839	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ S)5d	² D	5/2	1.09 × 10 ⁸	1.52 × 10 ⁸
7	1239.72	1239.738	−0.018	80,663	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	2.01 × 10 ⁷	4.27 × 10 ⁷ *
9	1252.01	1252.014	−0.004	79,872	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ S)5d	² D	5/2	8.27 × 10 ⁷	1.89 × 10 ⁸ *
9	1257.30	1257.309	−0.010	79,535	4s ² 4p ² (³ P)5p	² S	1/2	−	4s ² 4p ² (¹ D)5d	² P	3/2	4.62 × 10 ⁶	6.83 × 10 ⁶ *
12w	1334.04	1334.035	0.005	74,960	4s ² 4p ² (³ P)5p	⁴ D	3/2	−	4s ² 4p ² (¹ D)5d	² D	5/2	8.59 × 10 ⁶	6.72 × 10 ⁶ *
9	1366.05	1366.054	−0.004	73,204	4s ² 4p ² (¹ D)5p	² D	3/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	1.10 × 10 ⁷	1.95 × 10 ⁷ *
11	1371.72	1371.696	0.024	72,901	4s ² 4p ² (¹ D)5p	² F	5/2	−	4s ² 4p ² (¹ S)5d	² D	5/2	9.20 × 10 ⁶	3.05 × 10 ⁶ *
2d	1373.71	1373.705	0.005	72,796	4s ² 4p ² (¹ D)5p	² D	5/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	8.33 × 10 ⁶	8.31 × 10 ⁶ *
8	1397.90	1397.910	−0.010	71,536	4s ² 4p ² (¹ D)5p	² F	7/2	−	4s ² 4p ² (¹ S)5d	² D	5/2	1.70 × 10 ⁶	2.94 × 10 ⁶
13	1402.88	1402.882	−0.002	71,282	4s ² 4p ² (¹ D)5p	² D	5/2	−	4s ² 4p ² (¹ S)5d	² D	5/2	5.62 × 10 ⁷	7.45 × 10 ⁷ *
10	1416.88	1416.894	−0.014	70,578	4s ² 4p ² (³ P)5p	⁴ D	5/2	−	4s ² 4p ² (¹ D)5d	² G	7/2	5.35 × 10 ⁶	3.00 × 10 ⁶ *
1d	1422.29	1422.281	0.009	70,309	4s ² 4p ² (³ P)5p	⁴ D	5/2	−	4s ² 4p ² (¹ D)5d	² F	5/2	1.83 × 10 ⁷	1.65 × 10 ⁷ *
3d	1430.68	1430.678	0.000	69,897	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (¹ D)5d	² P	3/2	1.08 × 10 ⁸	1.36 × 10 ⁸
3	1441.73	1441.695	0.035	69,361	4s ² 4p ² (³ P)5p	⁴ S	3/2	−	4s ² 4p ² (¹ D)5d	² S	1/2	3.16 × 10 ⁶	2.11 × 10 ⁶ *
10	1446.37	1446.342	0.028	69,139	4s ² 4p ² (³ P)5p	⁴ P	1/2	−	4s ² 4p ² (¹ D)5d	² P	1/2	2.48 × 10 ⁵	1.28 × 10 ⁶ *

Table 1. Cont.

9	1451.64	1451.672	−0.032	68,888	4s ² 4p ² (³ P)5p	² S	1/2	−	4s ² 4p ² (³ P)5d	² D	3/2	2.88 × 10 ⁷	2.13 × 10 ⁷ *
10	1454.25	1454.264	−0.010	68,764	4s ² 4p ² (³ P)5p	⁴ D	5/2	−	4s ² 4p ² (¹ D)5d	² F	7/2	1.69 × 10 ⁶	6.99 × 10 ⁵ *
10	1454.25	1454.249	0.000	68,764	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (¹ D)5d	² D	5/2	5.61 × 10 ⁸	5.58 × 10 ⁸
10	1461.99	1462.007	−0.017	68,400	4s ² 4p ² (¹ D)5p	² P	1/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	4.55 × 10 ⁷	1.81 × 10 ⁷ *
2d	1484.23	1484.229	0.001	67,375	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (¹ D)5d	² G	7/2	1.17 × 10 ⁵	1.85 × 10 ⁴ *
9	1484.74	1484.721	0.019	67,352	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (¹ D)5d	² G	7/2	1.36 × 10 ⁷	6.87 × 10 ⁶ *
8	1489.84	1489.832	0.008	67,121	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (¹ D)5d	² G	9/2	1.36 × 10 ⁴	2.58 × 10 ⁵ *
10	1490.17	1490.142	0.028	67,106	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (¹ D)5d	² F	5/2	1.19 × 10 ⁵	2.77 × 10 ⁵ *
9	1490.64	1490.638	0.002	67,085	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (¹ D)5d	² F	5/2	1.59 × 10 ⁸	2.12 × 10 ⁸ *
7	1519.70	1519.712	−0.012	65,802	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² S	1/2	2.18 × 10 ⁸	2.43 × 10 ⁸
10w	1525.27	1525.287	−0.017	65,562	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (¹ D)5d	² F	7/2	1.40 × 10 ⁷	1.60 × 10 ⁷ *
2d	1527.99	1528.009	−0.019	65,445	4s ² 4p ² (³ P)5p	⁴ D	3/2	−	4s ² 4p ² (³ P)5d	² D	3/2	7.96 × 10 ⁶	9.46 × 10 ⁶ *
10	1532.86	1532.885	−0.020	65,237	4s ² 4p ² (³ P)5p	⁴ D	3/2	−	4s ² 4p ² (³ P)5d	² D	5/2	9.49 × 10 ⁶	1.49 × 10 ⁷ *
10	1533.84	1533.834	0.006	65,196	4s ² 4p ² (³ P)5p	² S	1/2	−	4s ² 4p ² (³ P)5d	² P	1/2	6.85 × 10 ⁸	7.06 × 10 ⁸
4	1536.58	1536.598	−0.018	65,080	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (¹ D)5d	² S	1/2	1.16 × 10 ⁸	1.17 × 10 ⁸
7d	1538.82	1538.828	−0.008	64,985	4s ² 4p ² (³ P)5p	² S	1/2	−	4s ² 4p ² (³ P)5d	⁴ P	1/2	9.25 × 10 ⁵	4.51 × 10 ⁶ *
2d	1557.86	1557.897	−0.037	64,191	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² P	3/2	7.24 × 10 ⁷	1.80 × 10 ⁸ *
8	1561.93	1561.922	0.010	64,023	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ D)5d	² D	5/2	5.38 × 10 ⁸	7.16 × 10 ⁸
10	1575.66	1575.646	0.010	63,465	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (¹ D)5d	² P	3/2	1.06 × 10 ⁸	1.89 × 10 ⁸
5	1597.09	1597.128	−0.038	62,614	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ D)5d	² G	7/2	5.93 × 10 ⁷	4.68 × 10 ⁷ *
4d	1599.14	1599.143	−0.003	62,534	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² P	1/2	5.22 × 10 ⁵	2.00 × 10 ⁶ *
20w	1600.72	1600.710	0.010	62,472	4s ² 4p ² (³ P)5p	⁴ D	5/2	−	4s ² 4p ² (³ P)5d	² D	3/2	6.90 × 10 ⁶	7.53 × 10 ⁶ *
8	1603.99	1603.977	0.013	62,344	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ D)5d	² F	5/2	3.28 × 10 ⁸	4.76 × 10 ⁸
9	1615.20	1615.216	−0.016	61,912	4s ² 4p ² (³ P)5p	⁴ P	3/2	−	4s ² 4p ² (³ P)5d	² D	3/2	3.29 × 10 ⁸	3.49 × 10 ⁸
9	1615.88	1615.869	0.010	61,886	4s ² 4p ² (³ P)5p	² S	1/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	6.34 × 10 ⁸	6.13 × 10 ⁸
2d	1617.86	1617.850	0.010	61,810	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (¹ D)5d	² P	1/2	7.68 × 10 ⁷	8.58 × 10 ⁷
7d	1620.63	1620.665	−0.035	61,704	4s ² 4p ² (³ P)5p	⁴ P	3/2	−	4s ² 4p ² (³ P)5d	² D	5/2	1.00 × 10 ⁶	4.66 × 10 ⁶ *
3d	1629.27	1629.260	0.010	61,377	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² F	5/2	8.66 × 10 ⁷	1.02 × 10 ⁸ *
10	1644.78	1644.770	0.010	60,798	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (¹ D)5d	² F	7/2	8.72 × 10 ⁶	3.17 × 10 ⁶ *
10	1670.79	1670.798	−0.008	59,852	4s ² 4p ² (¹ D)4d	² G	9/2	−	4s ² 4p ² (¹ D)5p	² F	7/2	3.44 × 10 ⁹	3.74 × 10 ⁹
9	1671.80	1671.816	−0.016	59,816	4s ² 4p ² (³ P)5p	² D	3/2	−	4s ² 4p ² (³ P)5d	² D	3/2	6.59 × 10 ⁸	6.75 × 10 ⁸
9	1687.23	1687.227	0.000	59,269	4s ² 4p ² (³ P)5p	⁴ D	1/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	7.19 × 10 ⁸	6.97 × 10 ⁸
2	1687.80	1687.818	−0.018	59,249	4s ² 4p ² (³ P)5p	⁴ P	5/2	−	4s ² 4p ² (³ P)5d	² D	3/2	7.34 × 10 ⁷	8.58 × 10 ⁷
2d	1690.54	1690.535	0.005	59,153	4s ² 4p ² (¹ D)4d	² G	7/2	−	4s ² 4p ² (¹ D)5p	² F	5/2	2.08 × 10 ⁹	1.92 × 10 ⁹
5	1711.03	1711.018	0.010	58,444	4s ² 4p ² (³ P)5p	⁴ D	3/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	7.21 × 10 ⁷	7.75 × 10 ⁷ *

Table 1. Cont.

9	1717.59	1717.587	0.003	58,221	4s ² 4p ² (³ P)5p	⁴ P	³ / ₂	−	4s ² 4p ² (³ P)5d	² P	¹ / ₂	2.09 × 10 ⁸	2.12 × 10 ⁸
8	1720.66	1720.679	−0.019	58,117	4s ² 4p ² (³ P)5p	⁴ D	⁵ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	⁵ / ₂	1.75 × 10 ⁸	1.80 × 10 ⁸ *
6	1735.48	1735.503	−0.023	57,621	4s ² 4p ² (¹ D)5p	² D	³ / ₂	−	4s ² 4p ² (¹ D)5d	² S	¹ / ₂	4.37 × 10 ⁸	4.03 × 10 ⁸
10	1751.25	1751.279	−0.029	57,102	4s ² 4p ² (³ P)5p	⁴ S	³ / ₂	−	4s ² 4p ² (³ P)5d	² D	³ / ₂	9.20 × 10 ⁷	9.09 × 10 ⁷
9	1771.27	1771.269	0.001	56,457	4s ² 4p ² (³ P)5p	⁴ P	¹ / ₂	−	4s ² 4p ² (³ P)5d	² P	¹ / ₂	5.48 × 10 ⁸	5.27 × 10 ⁸
2d	1777.92	1777.932	−0.012	56,245	4s ² 4p ² (³ P)5p	⁴ P	¹ / ₂	−	4s ² 4p ² (³ P)5d	⁴ P	¹ / ₂	4.51 × 10 ⁷	5.85 × 10 ⁷
8	1781.73	1781.731	−0.001	56,125	4s ² 4p ² (³ P)5p	² D	³ / ₂	−	4s ² 4p ² (³ P)5d	² P	¹ / ₂	3.67 × 10 ⁸	2.87 × 10 ⁸
1d	1788.47	1788.473	−0.003	55,914	4s ² 4p ² (³ P)5p	² D	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ P	¹ / ₂	2.21 × 10 ⁸	1.67 × 10 ⁸
4	1820.98	1821.005	−0.025	54,915	4s ² 4p ² (³ P)5p	⁴ D	⁷ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	⁵ / ₂	8.76 × 10 ⁸	8.68 × 10 ⁸
2d	1821.12	1821.117	0.000	54,911	4s ² 4p ² (³ P)5p	⁴ P	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	³ / ₂	5.58 × 10 ⁸	5.63 × 10 ⁸
9	1821.72	1821.746	−0.026	54,893	4s ² 4p ² (³ P)5p	⁴ P	⁵ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	⁵ / ₂	2.49 × 10 ⁹	2.46 × 10 ⁹
8	1828.94	1828.955	−0.020	54,676	4s ² 4p ² (¹ D)5p	² F	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² G	⁷ / ₂	6.35 × 10 ⁸	6.39 × 10 ⁸
2d	1834.59	1834.602	−0.012	54,508	4s ² 4p ² (³ P)5p	² D	⁵ / ₂	−	4s ² 4p ² (³ P)5d	² D	³ / ₂	1.21 × 10 ⁸	1.43 × 10 ⁸
10	1835.99	1835.983	0.007	54,466	4s ² 4p ² (¹ D)5p	² D	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² D	⁵ / ₂	4.95 × 10 ⁷	4.61 × 10 ⁶ *
10	1837.93	1837.942	−0.012	54,409	4s ² 4p ² (¹ D)5p	² F	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² F	⁵ / ₂	1.94 × 10 ⁸	2.32 × 10 ⁸ *
6	1839.86	1839.867	−0.007	54,352	4s ² 4p ² (¹ D)5p	² D	³ / ₂	−	4s ² 4p ² (¹ D)5d	² P	¹ / ₂	9.20 × 10 ⁸	9.35 × 10 ⁸
10	1841.66	1841.635	0.025	54,299	4s ² 4p ² (³ P)5p	² D	⁵ / ₂	−	4s ² 4p ² (³ P)5d	² D	⁵ / ₂	1.09 × 10 ⁹	7.22 × 10 ⁸
2d	1856.66	1856.639	0.021	53,860	4s ² 4p ² (¹ D)5p	² D	³ / ₂	−	4s ² 4p ² (¹ D)5d	² D	³ / ₂	3.39 × 10 ⁹	3.26 × 10 ⁹
10	1867.74	1867.753	−0.013	53,541	4s ² 4p ² (³ P)5p	² P	³ / ₂	−	4s ² 4p ² (³ P)5d	² D	³ / ₂	8.85 × 10 ⁸	8.23 × 10 ⁸
10	1870.79	1870.801	−0.011	53,453	4s ² 4p ² (¹ D)5p	² D	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² D	³ / ₂	4.20 × 10 ⁸	4.37 × 10 ⁸
2	1872.27	1872.269	0.001	53,411	4s ² 4p ² (³ P)5p	⁴ S	³ / ₂	−	4s ² 4p ² (³ P)5d	² P	¹ / ₂	2.83 × 10 ⁶	2.39 × 10 ⁷ *
12	1873.53	1873.546	−0.016	53,375	4s ² 4p ² (³ P)5p	⁴ D	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ F	⁵ / ₂	7.41 × 10 ⁹	7.38 × 10 ⁹
11	1875.04	1875.043	−0.003	53,332	4s ² 4p ² (³ P)5p	² P	³ / ₂	−	4s ² 4p ² (³ P)5d	² D	⁵ / ₂	5.46 × 10 ⁹	5.68 × 10 ⁹
5	1875.89	1875.858	0.032	53,308	4s ² 4p ² (¹ D)5p	² F	⁷ / ₂	−	4s ² 4p ² (¹ D)5d	² G	⁷ / ₂	1.49 × 10 ⁹	1.97 × 10 ⁹
12	1879.71	1879.714	−0.004	53,200	4s ² 4p ² (³ P)5p	⁴ S	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ P	¹ / ₂	2.27 × 10 ⁹	2.25 × 10 ⁹
11	1879.85	1879.847	0.003	53,196	4s ² 4p ² (¹ D)5p	² D	³ / ₂	−	4s ² 4p ² (¹ D)5d	² F	⁵ / ₂	3.31 × 10 ⁹	3.12 × 10 ⁹
10	1881.59	1881.580	0.010	53,146	4s ² 4p ² (³ P)5p	⁴ P	¹ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	³ / ₂	1.88 × 10 ⁹	1.91 × 10 ⁹
12	1884.81	1884.817	−0.007	53,056	4s ² 4p ² (¹ D)5p	² F	⁷ / ₂	−	4s ² 4p ² (¹ D)5d	² G	⁹ / ₂	1.12 × 10 ¹⁰	1.38 × 10 ¹⁰
12	1884.82	1884.821	0.000	53,055	4s ² 4p ² (¹ D)5p	² D	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² G	⁷ / ₂	8.86 × 10 ⁹	8.78 × 10 ⁹
10	1885.31	1885.312	−0.002	53,042	4s ² 4p ² (¹ D)5p	² F	⁷ / ₂	−	4s ² 4p ² (¹ D)5d	² F	⁵ / ₂	1.37 × 10 ⁸	2.51 × 10 ⁸
11	1891.71	1891.703	0.007	52,862	4s ² 4p ² (¹ D)5p	² F	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² F	⁷ / ₂	9.39 × 10 ⁹	9.42 × 10 ⁹
11	1893.31	1893.323	−0.013	52,818	4s ² 4p ² (³ P)5p	² P	¹ / ₂	−	4s ² 4p ² (³ P)5d	² D	³ / ₂	2.34 × 10 ⁹	2.45 × 10 ⁹
10	1893.39	1893.390	0.000	52,815	4s ² 4p ² (³ P)5p	² D	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	³ / ₂	6.37 × 10 ⁸	6.42 × 10 ⁸
11	1894.38	1894.367	0.013	52,788	4s ² 4p ² (¹ D)5p	² D	⁵ / ₂	−	4s ² 4p ² (¹ D)5d	² F	⁵ / ₂	3.75 × 10 ⁹	3.88 × 10 ⁹
11	1895.87	1895.898	−0.028	52,746	4s ² 4p ² (³ P)5p	⁴ S	³ / ₂	−	4s ² 4p ² (³ P)5d	⁴ D	⁵ / ₂	3.07 × 10 ⁹	3.04 × 10 ⁹

Table 1. Cont.

10	1897.70	1897.687	0.013	52,695	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (³ P)5d	⁴ F	9/2	1.32 × 10 ¹⁰	1.32 × 10 ¹⁰
15w	1901.49	1901.454	0.036	52,590	4s ² 4p ² (¹ S)5p	² P	3/2	−	4s ² 4p ² (¹ S)5d	² D	3/2	5.81 × 10 ⁸	1.95 × 10 ⁷ *
10	1941.93	1941.923	0.007	51,495	4s ² 4p ² (¹ D)5p	² F	7/2	−	4s ² 4p ² (¹ D)5d	² F	7/2	1.15 × 10 ⁹	1.32 × 10 ⁹
5	1951.53	1951.531	−0.001	51,242	4s ² 4p ² (¹ D)5p	² D	5/2	−	4s ² 4p ² (¹ D)5d	² F	7/2	2.13 × 10 ⁷	2.77 × 10 ⁷ *
50w	1954.14	1954.181	−0.041	51,173	4s ² 4p ² (³ P)5p	² D	3/2	−	4s ² 4p ² (³ P)5d	⁴ P	5/2	1.56 × 10 ⁸	6.14 × 10 ⁸
10	1975.25	1975.209	0.041	50,626	4s ² 4p ² (³ P)5p	⁴ D	7/2	−	4s ² 4p ² (³ P)5d	⁴ P	5/2	1.78 × 10 ⁶	1.43 × 10 ⁶ *
12	1979.08	1979.125	−0.045	50,528	4s ² 4p ² (¹ D)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² S	1/2	9.50 × 10 ⁸	1.12 × 10 ⁹
7	1984.01	1984.034	−0.024	50,403	4s ² 4p ² (³ P)5p	⁴ D	5/2	−	4s ² 4p ² (³ P)5d	⁴ F	5/2	2.12 × 10 ⁸	2.26 × 10 ⁸ *
11	1993.92	1993.936	−0.016	50,152	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (³ P)5d	⁴ D	5/2	1.33 × 10 ⁹	1.35 × 10 ⁹
6	1995.93	1995.958	−0.028	50,102	4s ² 4p ² (³ P)5p	⁴ S	3/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	1.42 × 10 ⁵	3.26 × 10 ⁵ *
	λ_{obs}	λ_{Ritz}	$\lambda_{obs} - \lambda_{Ritz}$										
	Air(Å)	Air (Å)	Air (Å)										
3	2013.93	2013.907	0.023	49,638.1	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (³ P)5d	⁴ P	1/2	6.75 × 10 ⁶	6.90 × 10 ⁶
9ul	2017.63	2017.622	0.010	49,547.1	4s ² 4p ² (¹ D)5p	² P	1/2	−	4s ² 4p ² (¹ D)5d	² P	1/2	1.18 × 10 ⁹	1.17 × 10 ⁹
3	2034.88	2034.879	−0.003	49,127.3	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (³ P)5d	² P	1/2	4.00 × 10 ⁸	4.67 × 10 ⁸
9	2037.85	2037.818	0.027	49,055.7	4s ² 4p ² (¹ D)5p	² P	1/2	−	4s ² 4p ² (¹ D)5d	² D	3/2	6.09 × 10 ⁸	6.31 × 10 ⁸
2	2043.67	2043.680	−0.006	48,915.8	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (³ P)5d	⁴ P	1/2	8.84 × 10 ⁷	1.07 × 10 ⁸
1d	2060.14	2060.089	0.052	48,524.8	4s ² 4p ² (³ P)4d	⁴ P	3/2	−	4s ² 4p ² (³ P)5p	² P	1/2	5.21 × 10 ⁵	1.14 × 10 ⁶ *
7	2092.17	2092.188	−0.020	47,782.2	4s ² 4p ² (¹ D)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² D	5/2	2.59 × 10 ⁹	2.87 × 10 ⁹
7	2093.74	2093.783	−0.048	47,746.4	4s ² 4p ² (³ P)5p	² D	3/2	−	4s ² 4p ² (³ P)5d	⁴ F	5/2	1.66 × 10 ⁷	1.92 × 10 ⁷ *
2	2104.27	2104.247	0.026	47,507.3	4s ² 4p ² (³ P)5p	² D	5/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	4.52 × 10 ⁷	4.15 × 10 ⁷ *
4	2115.32	2115.331	−0.010	47,259.2	4s ² 4p ² (¹ D)5p	² P	3/2	−	4s ² 4p ² (¹ D)5d	² P	1/2	1.49 × 10 ⁸	1.27 × 10 ⁸
10	2148.01	2147.995	0.020	46,540.0	4s ² 4p ² (³ P)5p	² P	3/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	5.56 × 10 ⁸	5.62 × 10 ⁸
1d	2150.95	2150.963	−0.010	46,476.4	4s ² 4p ² (¹ D)4d	² G	7/2	−	4s ² 4p ² (³ P)5p	⁴ P	5/2	2.44 × 10 ⁷	2.09 × 10 ⁷
8	2152.00	2151.997	0.006	46,453.7	4s ² 4p ² (¹ D)4d	² G	7/2	−	4s ² 4p ² (³ P)5p	⁴ D	7/2	1.24 × 10 ⁵	1.06 × 10 ⁵ *
7	2156.20	2156.204	−0.002	46,363.3	4s ² 4p ² (¹ D)5p	² F	5/2	−	4s ² 4p ² (³ P)5d	² D	5/2	4.15 × 10 ⁹	4.36 × 10 ⁹
5	2181.91	2181.898	0.010	45,817.1	4s ² 4p ² (³ P)5p	² P	1/2	−	4s ² 4p ² (³ P)5d	⁴ D	3/2	2.27 × 10 ⁸	2.05 × 10 ⁸
1d	2183.42	2183.412	0.005	45,785.4	4s ² 4p ² (¹ D)4d	² G	9/2	−	4s ² 4p ² (³ P)5p	⁴ D	7/2	1.53 × 10 ⁷	1.32 × 10 ⁷ *
5	2214.12	2214.132	−0.012	45,150.6	4s ² 4p ² (¹ D)5p	² D	3/2	−	4s ² 4p ² (³ P)5d	² D	5/2	2.14 × 10 ⁸	2.49 × 10 ⁸
1d	2221.75	2221.721	0.028	44,995.6	4s ² 4p ² (¹ D)5p	² F	7/2	−	4s ² 4p ² (³ P)5d	² D	5/2	4.23 × 10 ⁶	7.72 × 10 ⁶ *
2d	2223.96	2223.963	−0.005	44,950.9	4s ² 4p ² (¹ D)5p	² D	5/2	−	4s ² 4p ² (³ P)5d	² D	3/2	4.78 × 10 ⁷	5.69 × 10 ⁷
20	2259.70	2259.589	0.111	44,240.0	4s ² 4p ² (³ P)4d	⁴ P	3/2	−	4s ² 4p ² (³ P)5p	⁴ S	3/2	2.98 × 10 ⁸	2.72 × 10 ⁸
4	2399.16	2399.164	−0.004	41,668.6	4s ² 4p ² (¹ D)5p	² D	3/2	−	4s ² 4p ² (³ P)5d	² P	1/2	1.28 × 10 ⁸	1.06 × 10 ⁸
9	2465.05	2465.098	−0.044	40,554.8	4s ² 4p ² (¹ D)5p	² P	1/2	−	4s ² 4p ² (³ P)5d	² D	3/2	3.90 × 10 ⁸	3.86 × 10 ⁸
1	2587.91	2587.912	−0.002	38,629.6	4s ² 4p ² (¹ D)5p	² F	7/2	−	4s ² 4p ² (³ P)5d	⁴ F	9/2	8.88 × 10 ⁶	2.78 × 10 ⁶ *

Table 1. Cont.

4	2612.55	2612.525	0.025	38,265.3	4s ² 4p ² (¹ D)5p	² P	³ / ₂	–	4s ² 4p ² (³ P)5d	² D	³ / ₂	7.81 × 10 ⁷	6.89 × 10 ⁷
5	2701.33	2701.322	0.008	37,007.8	4s ² 4p ² (¹ S)5p	² P	³ / ₂	–	4s ² 4p ² (¹ D)5d	² S	¹ / ₂	2.92 × 10 ⁴	1.75 × 10 ⁷ *
1	2824.42	2824.418	0.002	35,395.0	4s ² 4p ² (¹ S)5p	² P	³ / ₂	–	4s ² 4p ² (¹ D)5d	² P	³ / ₂	2.93 × 10 ⁷	9.48 × 10 ⁷
1	2897.56	2897.578	−0.018	34,501.6	4s ² 4p ² (¹ D)5p	² F	⁵ / ₂	–	4s ² 4p ² (³ P)5d	⁴ F	⁵ / ₂	4.34 × 10 ⁶	4.21 × 10 ⁶
5	2948.13	2948.118	0.012	33,909.8	4s ² 4p ² (¹ D)5p	² P	³ / ₂	–	4s ² 4p ² (³ P)5d	⁴ D	⁵ / ₂	2.54 × 10 ⁶	1.91 × 10 ⁶ *
1	2979.38	2979.384	−0.004	33,554.2	4s ² 4p ² (¹ D)5p	² P	¹ / ₂	–	4s ² 4p ² (³ P)5d	⁴ D	³ / ₂	1.01 × 10 ⁷	8.11 × 10 ⁶ *
1	3006.77	3006.775	−0.005	33,248.5	4s ² 4p ² (¹ S)5p	² P	³ / ₂	–	4s ² 4p ² (¹ D)5d	² D	³ / ₂	1.08 × 10 ⁷	8.76 × 10 ⁶
2	3068.13	3068.139	−0.009	32,583.6	4s ² 4p ² (¹ S)5p	² P	³ / ₂	–	4s ² 4p ² (¹ D)5d	² F	⁵ / ₂	2.60 × 10 ⁵	5.35 × 10 ⁶ *
4	3626.08	3626.113	−0.033	27,570.1	4s ² 4p ² (³ P)4d	² P	¹ / ₂	–	4s ² 4p ² (³ P)5p	² P	¹ / ₂	2.16 × 10 ⁷	1.47 × 10 ⁷
2	3723.81	3723.780	0.030	26,846.5	4s ² 4p ² (³ P)4d	² P	¹ / ₂	–	4s ² 4p ² (³ P)5p	² P	³ / ₂	3.17 × 10 ⁷	3.37 × 10 ⁷
3	3816.34	3816.323	0.017	26,195.6	4s ² 4p ² (¹ D)5p	² P	³ / ₂	–	4s ² 4p ² (³ P)5d	⁴ F	⁵ / ₂	1.72 × 10 ⁵	1.63 × 10 ⁵ *
6	3873.25	3873.249	0.001	25,810.8	4s ² 4p ² (¹ D)4d	² S	¹ / ₂	–	4s ² 4p ² (³ P)5p	² P	¹ / ₂	1.74 × 10 ⁷	2.30 × 10 ⁷
1	4039.87	4039.870	0.002	24,746.2	4s ² 4p ² (¹ S)5p	² P	³ / ₂	–	4s ² 4p ² (³ P)5d	² D	³ / ₂	1.64 × 10 ⁶	1.95 × 10 ⁵ *

w: this line appeared wider than the others in our experiment; d: the line contour does not appear very clearly on our plate, increasing the error in the measurement; and ul is shaded to longer wavelengths. * Refers to lines with a cancellation factor less than 0.05.

3. Spectral Analysis and Theoretical Interpretation

To help in the spectral analysis, we calculated the level structures, the energy level lifetimes (τ), and weighted transition probabilities (gA) with the Hartree–Fock Cowan’s package [15] corrected by Kramida [23,24] and downloaded from the NIST website [25]. The programs that we used were modified as described by Pagan et al. [16] to include core polarization effects [26–28]. These methods demand knowledge of the polarizability and core cut radius. In this case, for Kr IV, a dipole polarizability $\alpha_d = 0.20 a_0^3$ and a cut off radius $r_c = 0.55 a_0$ were taken from references [13,29], corresponding to a Kr⁸⁺ closed shell ionic core of the type 1s²2s²2p⁶3s²3p⁶3d¹⁰, while the latter value was chosen as the mean value of $\langle r \rangle$ for the outer most core orbital (3d), as calculated by the HFR approach. We adjusted the values of the energy parameters to the experimental energy levels of this ion using a least squares calculation. With the adjusted values, we calculated the energy and composition of the levels as well as the gA and lifetimes of the energy levels [9,15]. The set of configurations for both of the parities used in our calculation was 4s²4p³ + 4s²4p²5p + 4s²4p²6p + 4s²4p²4f + 4s²4p²5f + 4s²4p²6f + 4s4p³4d + 4s4p³5d + 4s4p³6d + 4s4p³5s + 4s4p³6s + 4s²4p4d² + 4s²4p4f² + 4p⁵ + 4p⁴4f (odd parity) and 4s4p⁴ + 4s²4p²4d + 4s²4p²5d + 4s²4p²6d + 4s²4p²5s + 4s²4p²6s + 4s²4p²7s + 4s4p³4f + 4s4p³5f + 4s4p³6f + 4s4p³5p + 4s4p³6p + 4p⁴4d + 4p⁴5s + 4s4p²4d² (even parity). Intravalence correlations were considered in this calculation compared to previous work [2,9], where fewer configurations were taken into account. The introduction of the Rydberg series CI reduced the discrepancy between the observed and calculated levels values. Table 2 shows the new experimental and fitted energy level values obtained by the least-squares fit with the percentage composition in LS notation. We extended the analysis of reference [2], presenting five and twenty new energy levels for the 4s²4p²4d and 4s²4p²5d configurations respectively. Additionally, the lifetimes of the energy levels calculated with HFR were reported by taking the fitted energy parameters and HFR + CP effects into account, as shown in the last two columns of this table. Table 1 shows 168 new classified lines of Kr IV that were classified using the new levels presented in this work, where the intensities of the lines given in the table were based on visual estimates of plate blackening. This table also reports the Ritz wavelength and its difference to observed values, calculated with

the LOPT program [21]. The classification of the lower and the upper levels is presented. With the exception of transitions involving $J = 9/2$, it can be seen from this table that more than four spectral lines determine each experimental level. For example, in the best case, the level $4s^24p^2(^3P)5d\ ^2D_{3/2}$ in $303,713.2\text{ cm}^{-1}$ is determined by 17 transitions. The gA values in this table are from HFR and HFR + CP calculations, made with energy parameters adjusted by least-squares fitting. The label “*” in the last column refers to lines with cancellation factors [9] less than 0.05, as this fact may reflect errors in the estimation of gA values [15]. The least-squares calculation results are shown in Table 3 for even parity. The average energies (E_{av}) for the observed energy levels, the spin-orbit integrals (ζ_{nl}), and the single-configuration Slater integrals (F^k, G^k) were adjusted, keeping them free in the calculation except for the $G^1(4p,5s)$ of the $4s^24p^25s$ configuration, which was fixed at 85% at its HF value. The α_d values for the $4s^24p^25d$, $4s^24p^25s$ and $4s^24p^26s$ configurations were also fixed in the calculation. The configuration interactions $4s4p^4-4s^24p^24d$ ($R^1(4p4p,4s4d)$) and $4s4p^4-4s^24p^25d$ ($R^1(4p4p,4s5d)$) were kept free, but the CI integrals omitted in this table were set to 85% of their HFR values, and the direct and exchange integral, and spin-orbit ζ parameters were set to 85% and 95% of their HFR values. The standard deviation for the energy adjustment was 266 cm^{-1} .

Table 2. New Kr IV energy levels.

Configuration	Term	J	Observed Levels (cm^{-1})	Fitted ^a (cm^{-1})	Composition ^b	Lifetimes (ns)	
						HFR	HFR + CP
$4s^24p^2(^1D)4d$	2G	$7/2$	197,989.6	198,019	95	4.313	4.586
$4s^24p^2(^1D)4d$	2G	$9/2$	198,657.9	198,836	95	∞ ^c	∞ ^c
$4s^24p^2(^3P)4d$	4P	$3/2$	202,370.6	202,488	$64\ 4s^24p^2(^3P)4d^4P + 15\ 4s^24p^2(^3P)5s^4P$	0.027	0.030
$4s^24p^2(^3P)4d$	2P	$1/2$	223,326.7	223,286	$43\ 4s^24p^2(^1D)4d^2P + 17\ 4s^24p^2(^3P)4d^2P + 17\ 4s^24p^2(^1D)4d^2S$	0.032	0.034
$4s^24p^2(^1D)4d$	2S	$1/2$	225,085.8	225,565	$35\ 4s^24p^2(^1D)4d^2S + 18\ 4s^24p^2(^1S)5s^2S + 12\ 4s4p^4(^1S)2S$	0.031	0.034
$4s^24p^2(^3P)5d$	4F	$5/2$	291,643.9	291,613	$53\ 4s^24p^2(^3P)5d^4F + 24\ 4s^24p^2(^3P)5d^4D + 6\ 4s^24p^2(^3P)5d^4P$	0.411	0.487
$4s^24p^2(^3P)5d$	4P	$5/2$	295,071.0	295,054	$38\ 4s^24p^2(^3P)5d^4P + 37\ 4s^24p^2(^3P)5d^4F + 15\ 4s^24p^2(^3P)5d^4D$	0.251	0.324
$4s^24p^2(^3P)5d$	4D	$3/2$	296,713.9	296,708	$34\ 4s^24p^2(^3P)5d^2P + 30\ 4s^24p^2(^3P)5d^4D + 20\ 4s^24p^2(^3P)5d^4P$	0.250	0.317
$4s^24p^2(^3P)5d$	4F	$9/2$	297,139.1	297,235	$92\ 4s^24p^2(^3P)5d^4F + 64\ 4s^24p^2(^1D)5d^2G$	0.644	0.672
$4s^24p^2(^3P)5d$	4D	$5/2$	299,358.1	299,238	$55\ 4s^24p^2(^3P)5d^4D + 28\ 4s^24p^2(^3P)5d^4P + 6\ 4s^24p^2(^1D)5d^2D$	0.265	0.341
$4s^24p^2(^3P)5d$	4P	$1/2$	299,812.3	299,736	81	0.177	0.248
$4s^24p^2(^3P)5d$	2P	$1/2$	300,023.8	300,106	$63\ 4s^24p^2(^3P)5d^2P + 13\ 4s^24p^2(^3P)5d^4D + 13\ 4s^24p^2(^3P)6s^2P$	0.269	0.314
$4s^24p^2(^3P)5d$	2D	$5/2$	303,505.7	303,483	$77\ 4s^24p^2(^3P)5d^2D + 12\ 4s^24p^2(^1D)5d^2F$	0.166	0.222
$4s^24p^2(^3P)5d$	2D	$3/2$	303,713.8	303,523	$77\ 4s^24p^2(^3P)5d^2D + 54\ 4s^24p^2(^1D)5d^2D$	0.182	0.228
$4s^24p^2(^1D)5d$	2F	$7/2$	310,004.9	310,016	$60\ 4s^24p^2(^1D)5d^2F + 32\ 4s^24p^2(^1D)5d^2G$	0.296	0.369
$4s^24p^2(^1D)5d$	2F	$5/2$	311,551.1	311,455	$37\ 4s^24p^2(^1D)5d^2F + 33\ 4s^24p^2(^1D)5d^2D + 7\ 4s^24p^2(^3P)6d^2F$	0.183	0.228
$4s^24p^2(^1D)5d$	2G	$9/2$	311,565.1	311,277	$94\ 4s^24p^2(^1D)5d^2G + 6\ 4s^24p^2(^3P)5d^4F$	0.629	0.657
$4s^24p^2(^1D)5d$	2G	$7/2$	311,818.5	312,038	$57\ 4s^24p^2(^1D)5d^2G + 21\ 4s^24p^2(^1D)5d^2F + 14\ 4s^24p^2(^3P)5d^2F$	0.275	0.320
$4s^24p^2(^1D)5d$	2D	$3/2$	312,216.1	312,118	82	0.165	0.219
$4s^24p^2(^1D)5d$	2P	$1/2$	312,707.1	313,106	91	0.254	0.326
$4s^24p^2(^1D)5d$	2D	$5/2$	313,229.8	313,112	$49\ 4s^24p^2(^1D)5d^2D + 15\ 4s^24p^2(^1D)5d^2F + 10\ 4s^24p^2(^3P)5d^2D$	0.186	0.220
$4s^24p^2(^1D)5d$	2P	$3/2$	314,362.6	313,986	$48\ 4s^24p^2(^1D)5d^2P + 26\ 5s5p^3(^4S)5p^4P$	0.305	0.266
$4s^24p^2(^1D)5d$	2S	$1/2$	315,975.5	316,136	$72\ 4s^24p^2(^1D)5d^2S + 6\ 5s5p^3(^4S)5p^4P$	0.224	0.255
$4s^24p^2(^1S)5d$	2D	$5/2$	330,044.9	330,452	$82\ 4s^24p^2(^1S)5d^2D + 8\ 4s^24p^2(^3P)6d^2D$	0.225	0.334
$4s^24p^2(^1S)5d$	2D	$3/2$	331,558.9	331,141	$74\ 4s^24p^2(^1S)5d^2D + 8\ 4s^24p^2(^3P)6d^2D$	0.173	0.271

^a Calculated energy level values obtained using the fitted energy parameters. ^b Percentages below 5% have been omitted. ^c Lifetime is infinite for electric dipole (E1) transitions.

Table 3. Energy parameters (cm^{-1}) for the studied even parity configurations of Kr IV.

Configuration	Parameter	H-F Value	Fitted Value	Fitt/H-F ^a
4s4p ⁴	E _{av}	139,218	167,777 ± 292	1.20
	F ² (4p,4p)	63,178	57,606 ± 833	0.91
	α		−135 ± 75	
	ζ _{4p}	4190	4151 ± 308	0.99
4s ² 4p ² 4d	G ¹ (4s,4p)	85,055	71,598 ± 464	0.84
	E _{av}	178,106	206,020 ± 924	1.16
	F ² (4p,4p)	64,225	51,349 ± 924	0.80
	α		127 ± 45	
	ζ _{4p}	4373	4649 ± 147	1.06
	ζ _{4d}	208	198(FIX)	0.95
	F ² (4p,4d)	46,830	41,477 ± 734	0.88
	G ¹ (4p,4d)	55,585	46,768 ± 277	0.84
4s ² 4p ² 5d	G ³ (4p,4d)	34,132	28,337 ± 724	0.83
	E _{av}	285,175	304,785 ± 75	1.07
	F ² (4p,4p)	65,623	50,322 ± 477	0.77
	α		40(FIX)	
	ζ _{4p}	4568	4827 ± 152	1.06
	ζ _{5d}	68	65(FIX)	0.95
	F ² (4p,5d)	12,907	10,007 ± 528	0.77
	G ¹ (4p,5d)	9487	7048 ± 351	0.74
	G ³ (4p,5d)	6483	4164 ± 590	0.64
	E _{av}	195,483	218,447 ± 168	1.12
4s ² 4p ² 5s	F ² (4p,4p)	65,132	51,051 ± 1455	0.78
	α		0(FIX)	
	ζ _{3p}	4521	3059 ± 287	0.67
	G ¹ (4p,5s)	6596	5607(FIX)	0.85
	E _{av}	289,383	309,075 ± 121	1.07
	F ² (4p,4p)	65,686	52,182 ± 1477	0.79
4s ² 4p ² 6s	α		0(FIX)	
	ζ _{3p}	4586	4417 ± 232	0.96
	G ¹ (4p,6s)	2023	1390 ± 368	0.69
Configuration Interaction Integrals				
4s4p ⁴ –4s ² 4p ² 4d	R ¹ (4p4p,4s4d)	66,568	57,280 ± 381	0.86
4s4p ⁴ –4s ² 4p ² 5d	R ¹ (4p4p,4s5d)	27,412	23,228 ± 2428	0.85

^a Parameters omitted from this table: direct and exchange integrals and spin-orbit ζ parameters set to 85% and 95% of their HFR values respectively; CI integrals were set to 85% of their HFR values. The standard deviation for the energy adjustment was 266 cm^{-1} .

4. Conclusions

We studied the Kr IV spectrum covering the wavelength range 330–4800 Å using a capillary-pulsed discharge and a theta-pinch. We extended the analysis of this ion, including five energy levels of the configuration 3s²3p²4d and twenty levels of the 3s²3p²5d configuration. A total of 168 spectral lines were classified for the first time. Atomic HFR and HFR + CP calculation to determine weighted transition rates (gA) for all experimentally observed lines and lifetimes for new energy levels were used.

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