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New energy levels of the $4s^24p5s$, $4s^24p4d$ and $4s^24p5p$ configurations of the Kr v spectrum

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Abstract

The spectrum of four-times-ionized krypton (Kr v) has been observed in the 240–2500 Å wavelength range. Three of the four possible levels of the $4s^24p5s$ configuration and two of the three remaining energy level values for the $4s^24p4d$ configurations were determined. Nine of the ten possible levels for the $4s^24p5p$ configuration are also reported. The observed configurations were interpreted theoretically by means of Hartree–Fock relativistic calculations and a least-squares fit of the energy parameters to the observed levels. 111 new classified lines are reported among the $4s^24p^2$, $4s^24p5p$, $4s4p^3$, $4s^24p5s$, and $4s^24p4d$ configurations.

1. Introduction

Energy levels of Kr I to Kr XXXVI were reviewed and compiled by Sugar and Musgrove (1991) and tables of the classified lines of Kr v to Kr XXXVI were compiled by Shirai *et al* (1995).

Four-times-ionized krypton, Kr v, belongs to the Ge I isoelectronic sequence and has the ground configuration $4s^24p^2$. The spectra of the first, second, third and fourth elements of this sequence were presented in the book *Atomic Energy Levels* (Moore 1971). The As II spectrum was reinvestigated by Li and Andrew (1971) and the Br IV spectrum was revised by Joshi and Budhiraja (1971).

The krypton isonuclear sequence has also been studied in different works by members of the Centro de Investigaciones Opticas Group, La Plata, Argentina and the Campinas Group, São Paulo, Brazil. Reyna Almandos *et al* (1996, 1998) published new energy levels for Kr III and Kr IV. Pagan *et al* (1995) reported the study of the 4s4p4d and 4s4p5s configurations of Kr VI and Raineri *et al* (2000) presented the spectroscopic analysis of the 4p4d configuration of Kr VII. All these experiments were carried out using a discharge tube and a theta-pinch discharge.

Trigueiros *et al* (1989, 1993), and references therein, studied the Kr v spectrum using different spectral sources. These authors presented new energy levels of the $4s^24p^2$, $4s4p^3$, $4s^24p4d$ and $4p^4$ configurations.

In this work we report an extended analysis of the four-times-ionized krypton (Kr v). We have established three new energy levels for the $4s^24p5s$, two for the $4s^24p4d$ and nine for the $4s^24p5p$ configurations. 111 new lines were classified as combinations between levels of $4s^24p^2$, $4s^24p5p$, $4s4p^3$, $4s^24p5s$, and $4s^24p4d$ configurations. Analysis of the experimental data used Hartree–Fock calculation and parametric fit.

Configurations of the type $ns^2npn'p$ have been studied by Kramida *et al* (1999) ($n = 2$, $n' = 3$) and Gallardo *et al* (1999) ($n = 5$, $n' = 6$) for elements of the same homologous sequence.

The interest in spectroscopic data for rare gases is due to applications in collision physics, laser physics, photo-electron spectroscopy and fusion diagnostics.

2. Experiment

The work is based on photographic recordings of the spectra of krypton between 240 and 2500 Å. We have used two different light sources in our experiment, a discharge tube and a theta-pinch discharge. In both cases the energy is fed into the plasma using a capacitor bank, charged from a high-voltage power supply. The discharge tube was built at the Centro de Investigaciones Opticas (CIOp), La Plata, Argentina, to study highly ionized gases (Gallardo *et al* 1989). It is made with a Pyrex tube ending in a quartz window. The electrodes, 20 cm apart, were made of tungsten and covered with indium. The gas pressure was measured by a thermocouple vacuum gauge before and after exposures. The pressure range was varied between 20 and 300 mTorr. Gas excitation was produced by discharging through the tube a bank of low-inductance capacitors varying between 2.5 and 100 nF and charged up to 19 kV. A normal-incidence vacuum spectrograph with a concave diffraction grating of 1200 lines mm^{-1} was used. The plate factor in the first order is 2.77 Å mm^{-1}. Kodak SWR plates were used to record the spectra. C III, N II and N III (Kelly 1987), O III (Pettersson 1982) and known lines of krypton (Kelly 1987, Shirai *et al* 1995, Raineri *et al* 1998) were recorded as internal standard lines.

The other experimental data were obtained several years ago by two of the authors (JRA and AGT) at the Lund Institute of Technology, Sweden, using the theta pinch discharge. This consisted primarily of a cylindrical discharge tube, excited by an induction coil. The spark gap was pressurized with air. It was ignited by lowering the pressure in the spark chamber by means of a magnetic valve and triggered when the capacitor voltage reached a preset value. The theta pinch device had the following specifications: total capacitance 7.7 μF, total inductance 76 nH, period of damped oscillation 4.8 μs. Maximum current at 10 kV discharge voltage is about 100 kA. The repetition rate of the discharge was about 15 min^{-1} at a capacitor bank voltage of 10 kV. A 3 m normal-incidence vacuum spectrograph with a concave diffraction grating of 1200 lines mm^{-1} was used. The plate factor in the first order was 2.77 Å mm^{-1}. The spectra were exposed on Kodak SWR plates and the lines from C III, N II and N III (Kelly 1987), O III (Pettersson 1982) and known lines of krypton (Kelly 1987) were used as internal standards.

To distinguish between different states of ionization in both spectral sources, a number of experimental parameters, e.g., gas pressure, discharge voltage, capacitance and the number of discharges were varied (Gallardo *et al* 1989, Trigueiros *et al* 1989). The approximate total number of Kr lines for all stages observed over the pertinent wavelength range was 7500. The accuracy of the wavelength values is estimated to be ±0.01 and ±0.02 Å in the measurements of Lund and La Plata respectively.

3. Analysis

The line identifications were guided by theoretical predictions of the energy level structure and line strengths obtained from the Cowan (1981) computer code, using Hartree–Fock relativistic (HFR) wavefunctions.

The new Kr v classified lines observed in the present work are given in table 1. The intensities of the lines are based on visual estimates and the wavenumber values in the calculated column are derived from the experimental energy level values, which, in turn, were derived from the observed lines. The predicted wavelength and log gf values, shown in columns 3 and 4 of this table, were obtained considering the fitted values for the energy parameters, in the HF calculation. This kind of calculation was also used to obtain the values of weighted oscillator strengths for Kr III and Kr IV spectra (Raineri *et al* 1998, Bredice *et al* 2000).

The new energy level values derived from the observed lines belonging to the 4s^{2}4p5p, 4s^{2}4p4d and 4s^{2}4p5s configurations are given in table 2. The energy level values were determined from the observed wavelengths. In our case the uncertainties of the adjusted experimental energy level values are generally less than 2 cm^{-1}. All level designations in table 2 are in LS notation, and in the same table we present the percentage composition of the levels that were taken from the least-squares fit.

The configuration set used in the calculation was 4s^{2}4p^2, 4s^{2}4p5p, 4s4p^{2}4d, 4p^4 and 4s^{2}4p4f for the even parity and 4s4p^3, 4s^{2}4p4d and 4s^{2}4p5s for the odd parity.

(i) $4s^24p4d$. The 4s^{2}4p4d configuration was studied by Trigueiros *et al* (1989). In this work we have extended the analysis reporting the new values 190 279 and 192 949 cm^{-1} for the ^{3}F$_2$ and ^{3}F$_3$ energy levels respectively. These levels were found by transitions with the new 4s^{2}4p5p and ground configurations. The theoretical value for the remaining ^{3}F$_4$ energy level of the 4s^{2}4p4d configuration obtained from the least-squares fit is 196 425 cm^{-1}.

(ii) $4s^24p5s$. We propose three new energy level values of this configuration. For the ^{3}P$_1$, ^{3}P$_2$ and ^{1}P$_1$ levels, the experimental values are 240 926, 246 798 and 250 993 cm^{-1} respectively. These levels were also found by transitions with the new 4s^{2}4p5p and ground configurations. The calculated value for the ^{3}P$_0$ energy level, obtained from the least-squares fit, is 238 871 cm^{-1}.

(iii) $4s^24p5p$. Of the ten possible levels of this configuration, we found nine of them by transitions with the 4s4p^3 and 4s^{2}4p4d configurations. Only the level 4s^{2}4p5p ^{3}P$_0$ was not determined. The theoretical value for this level obtained from the least-squares fit is 284 942 cm^{-1}. From the percentage composition of table 1, we can observe that the ^{3}D$_1$ and ^{1}P$_1$ levels are very mixed. In this case the LS designation has very little physical significance.

4. Theoretical interpretation

The configurations were interpreted by fitting the theoretical energy expression to the observed energy levels using least-squares techniques. The adjusted parameter values for the odd and even configurations are compared with results from HFR calculations in tables 3 and 4 respectively.

For the odd parity the matrix included the 4s4p^3 + 4s^{2}4p4d + 4s^{2}4p5s configurations. The fitted energy parameters were in accordance with scaled Hartree–Fock values. The effective electrostatic parameter α(4p, 4p) and the configuration interaction integral R^1(4p4p, 4s4d) between 4s4p^3 and 4s^{2}4p4d configurations were optimized and fixed in order to obtain better

Table 1. Classified lines of Kr v. Int: line intensities from visual estimation. Key to symbols: w, this line appeared wider than the others in our experiment; d, the line contour is not clear in our plate, increasing the error in the measurement; us, shaded to shorter wavelengths; ul, shaded to longer wavelengths. (,): these lines appeared blended.

Int. and shape[a]	λ_{obs} (Å)	λ_{pred} (Å)	Log gf	σ_{obs} (cm^{-1})	σ_{cal} (cm^{-1})[b]	Transition
12	2490.95	2495.11	−1.043	40 145	40 145	$4s^24p5p\ {}^3P_2-4s^24p5s\ {}^1P_1$
9	2426.80	2429.37	−0.267	41 206	41 207	$4s^24p5p\ {}^3D_1-4s^24p4d\ {}^1P_1$
20w	2387.50	2386.44	−0.596	41 885	41 885	$4s^24p5p\ {}^3P_1-4s^24p5s\ {}^3P_2$
10w	2341.13	2341.95	−0.911	42 714	42 712	$4s^24p5p\ {}^3S_1-4s^24p5s\ {}^1P_1$
50w	2339.19	2335.17	0.141	42 750	42 751	$4s^24p5p\ {}^3D_2-4s^24p5s\ {}^3P_1$
100w	2314.79	2316.24	0.475	43 200	43 200	$4s^24p5p\ {}^3D_3-4s^24p5s\ {}^3P_2$
100w	2255.34	2259.41	0.280	44 339	44 340	$4s^24p5p\ {}^3P_2-4s^24p5s\ {}^3P_2$
100w	2192.60	2190.33	0.290	45 608	45 607	$4s^24p5p\ {}^1D_2-4s^24p5s\ {}^1P_1$
20w	2181.60	2186.99	−0.659	45 838	45 838	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^1P_1$
50w	2176.02	2174.76	−0.194	45 955	45 956	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^1P_1$
20w	2131.83	2133.08	0.054	46 908	46 907	$4s^24p5p\ {}^3S_1-4s^24p5s\ {}^3P_2$
10	2007.96	2006.57	−0.869	49 802	49 802	$4s^24p5p\ {}^1D_2-4s^24p5s\ {}^3P_2$
9	1991.63	1993.77	−1.269[a]	50 210	50 212	$4s^24p5p\ {}^3P_2-4s^24p5s\ {}^3P_1$
11	1894.70	1894.75	−0.700	52 779	52 779	$4s^24p5p\ {}^3S_1-4s^24p5s\ {}^3P_1$
8	1796.21	1794.26	−1.629[a]	55 673	55 674	$4s^24p5p\ {}^1D_2-4s^24p5s\ {}^3P_1$
7	1789.65	1790.12	−2.806	55 877	55 877	$4s^24p5p\ {}^3D_3-4s^24p4d\ {}^1F_3$
6	1764.47	1765.43	−0.370	56 674	56 674	$4s^24p5p\ {}^1S_0-4s^24p5s\ {}^1P_1$
3	1698.42	1698.03	−0.778	58 878	58 879	$4s^24p5p\ {}^1D_2-4s^24p4d\ {}^1P_1$
10	1661.72	1657.07	−2.726[b]	60 179	60 181	$4s^24p5p\ {}^3D_1-4s^24p4d\ {}^3D_1$
10	1611.49	1616.72	−1.050	62 054	62 053	$4s^24p5p\ {}^3D_1-4s^24p4d\ {}^1D_2$
8	1599.82	1603.29	−2.786[b]	62 507	62 508	$4s^24p5p\ {}^3D_1-4s^24p4d\ {}^3P_0$
10	1568.91	1568.57	−1.279	63 738	63 736	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^3D_2$
9	1566.03	1562.27	−1.653	63 856	63 854	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^3D_2$
12w	1555.39	1555.69	−0.883	64 293	64 295	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^3D_3$
3d	1542.91	1540.61	−2.862[b]	64 813	64 812	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^3D_1$
15w	1540.07	1534.53	−3.522[b]	64 932	64 930	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^3D_1$
9	1538.55	1539.95	−1.294	64 996	64 995	$4s^24p5p\ {}^3D_1-4s^24p4d\ {}^3P_1$
5	1499.64	1505.67	−2.587[b]	66 683	66 684	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^1D_2$
2d	1498.28	1498.77	−1.876[b]	66 743	66 741	$4s^24p5p\ {}^1S_0-4s^24p5s\ {}^3P_1$
10ul	1452.26	1449.56	−1.564	68 858	68 860	$4s^24p5p\ {}^3P_1-4s^24p4d\ {}^3D_2$
10	1436.20	1438.86	−2.530[b]	69 628	69 626	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^3P_1$
10)	1433.78	1433.56	−1.551	69 746	69 744	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^3P_1$
15wul	1429.84	1425.65	−0.811	69 938	69 936	$4s^24p5p\ {}^3P_1-4s^24p4d\ {}^3D_1$
15wul	1429.84	1431.02	−4.565[b]	69 938	69 946	$4s^24p5p\ {}^1S_0-4s^24p4d\ {}^1P_1$
12w	1424.97	1423.36	−1.668	70 177	70 175	$4s^24p5p\ {}^3D_3-4s^24p4d\ {}^3D_2$
15w	1416.14	1417.90	−0.516	70 614	70 616	$4s^24p5p\ {}^3D_3-4s^24p4d\ {}^3D_3$
15	1402.20	1401.70	−0.360	71 316	71 315	$4s^24p5p\ {}^3P_2-4s^24p4d\ {}^3D_2$
14)	1393.61	1396.40	−0.197	71 756	71 756	$4s^24p5p\ {}^3P_2-4s^24p4d\ {}^3D_3$
15	1392.63	1395.68	−0.447	71 807	71 808	$4s^24p5p\ {}^3P_1-4s^24p4d\ {}^1D_2$
20	1384.59	1386.03	−0.379	72 223	72 222	$4s^24p5p\ {}^1P_1-4s^24p4d\ {}^3P_2$
9	1383.86	1385.66	−1.350	72 262	72 263	$4s^24p5p\ {}^3P_1-4s^24p4d\ {}^3P_0$
11	1382.35	1381.11	−1.170	72 341	72 340	$4s^24p5p\ {}^3D_2-4s^24p4d\ {}^3P_2$
8	1367.56	1371.37	−2.130	73 123	73 123	$4s^24p5p\ {}^3D_3-4s^24p4d\ {}^1D_2$
10	1337.77	1338.09	−1.932[b]	74 751	74 750	$4s^24p5p\ {}^3P_1-4s^24p4d\ {}^3P_1$
9)	1334.08	1331.19	−0.729	74 958	74 958	$4s^24p5p\ {}^3S_1-4s^24p4d\ {}^3D_1$
11	1302.43	1300.06	−1.258	76 780	76 777	$4s^24p5p\ {}^1D_2-4s^24p4d\ {}^3D_2$
10	1301.58	1305.03	−1.339	76 830	76 830	$4s^24p5p\ {}^3S_1-4s^24p4d\ {}^1D_2$

Table 1. (Continued.)

Int. and shape[a]	λ_{obs} (Å)	λ_{pred} (Å)	Log gf	σ_{obs} (cm^{-1})	σ_{cal} (cm^{-1})[c]	Transition
10	1295.08	1295.51	−1.291	77 215	77 218	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^3D_3$
(10	1292.87	1292.29	−0.992	77 347	77 346	$4s^24p5p\ ^3P_1$–$4s^24p4d\ ^3P_2$
7	1284.47	1280.80	−2.370	77 853	77 853	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^3D_1$
6d	1271.28	1271.42	-2.300^b	78 661	78 661	$4s^24p5p\ ^3D_3$–$4s^24p4d\ ^3P_2$
12w	1254.32	1256.55	−1.000	79 724	79 725	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^1D_2$
12	1253.54	1254.54	−0.881	79 774	79 772	$4s^24p5p\ ^3S_1$–$4s^24p4d\ ^3P_1$
10)	1253.12	1254.10	−1.022	79 801	79 801	$4s^24p5p\ ^3P_2$–$4s^24p4d\ ^3P_2$
10	1214.07	1214.19	−1.119	82 368	82 368	$4s^24p5p\ ^3S_1$–$4s^24p4d\ ^3P_2$
10	1209.63	1209.68	−1.886	82 670	82 667	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^3P_1$
7	1128.04	1129.30	−0.268	88 649	88 649	$4s^24p5p\ ^3D_1$–$4s^24p4d\ ^3F_2$
3d	1117.09	1117.40	−1.813	89 518	89 518	$4s^24p5p\ ^1P_1$–$4s4p^3\ ^1P_1$
12w	1102.19	1099.36	0.108	90 728	90 728	$4s^24p5p\ ^3D_2$–$4s^24p4d\ ^3F_3$
(12	1072.04	1073.97	−0.498	93 280	93 280	$4s^24p5p\ ^1P_1$–$4s^24p4d\ ^3F_2$
15w	1070.69	1071.01	−0.867	93 397	93 398	$4s^24p5p\ ^3D_2$–$4s^24p4d\ ^3F_2$
12	1030.40	1028.71	−0.841	97 050	97 049	$4s^24p5p\ ^3D_3$–$4s^24p4d\ ^3F_3$
11	1018.44	1017.35	−0.904	98 189	98 189	$4s^24p5p\ ^3P_2$–$4s^24p4d\ ^3F_3$
11	1016.22	1016.81	−1.041	98 404	98 404	$4s^24p5p\ ^3P_1$–$4s^24p4d\ ^3F_2$
5	1003.37	1002.96	-5.744^b	99 664	99 664	$4s^24p5p\ ^3S_1$–$4s4p^3\ ^1P_1$
20wus	1002.74	1003.85	−2.444	99 727	99 719	$4s^24p5p\ ^3D_3$–$4s^24p4d\ ^3F_2$
20wus	965.09	964.78	−1.784	103 617	103 619	$4s^24p5p\ ^3P_1$–$4s4p^3\ ^3S_1$
7	964.77	962.73	−1.770	103 652	103 651	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^3F_3$
2	940.55	940.92	−2.342	106 321	106 321	$4s^24p5p\ ^1D_2$–$4s^24p4d\ ^3F_2$
9	880.08	879.90	−0.807	113 626	113 626	$4s^24p5p\ ^1S_0$–$4s4p^3\ ^1P_1$
2	815.62	815.85	−0.572	122 606	122 603	$4s^24p5p\ ^1S_0$–$4s4p^3\ ^3S_1$
4d	767.69	768.03	−1.736	130 261	130 260	$4s^24p5p\ ^3D_1$–$4s4p^3\ ^3P_2$
8	767.35	767.75	−1.467	130 319	130 318	$4s^24p5p\ ^3S_1$–$4s4p^3\ ^1D_2$
50w	763.35	763.03	-3.652^b	131 001	131 003	$4s^24p5p\ ^3D_1$–$4s4p^3\ ^3P_0$
11	750.67	750.72	−0.583	133 214	133 213	$4s^24p5p\ ^1D_2$–$4s4p^3\ ^1D_2$
3d	707.56	707.87	−2.046	141 330	141 330	$4s^24p5p\ ^3D_3$–$4s4p^3\ ^3P_2$
9	701.9	702.47	−1.216	142 470	142 470	$4s^24p5p\ ^3P_2$–$4s4p^3\ ^3P_2$
10	689.47	689.77	−1.234	145 039	145 037	$4s^24p5p\ ^3S_1$–$4s4p^3\ ^3P_2$
9	687.66	687.71	−1.226	145 421	145 418	$4s^24p5p\ ^3S_1$–$4s4p^3\ ^3P_1$
4d	685.98	685.73	−1.683	145 777	145 780	$4s^24p5p\ ^3S_1$–$4s4p^3\ ^3P_0$
3d	676.00	675.99	-2.798^b	145 929	147 932	$4s^24p5p\ ^1D_2$–$4s4p^3\ ^3P_2$
6)	674.24	674.01	-3.251^b	148 315	148 313	$4s^24p5p\ ^1D_2$–$4s4p^3\ ^3P_1$
7	655.05	655.24	−1.177	152 660	152 661	$4s^24p5p\ ^3D_2$–$4s4p^3\ ^3D_3$
10	650.27	650.26	−1.046	153 782	153 780	$4s^24p5p\ ^1P_1$–$4s4p^3\ ^3D_2$
6	649.78	650.17	-2.361^b	153 898	153 900	$4s^24p5p\ ^1P_1$–$4s4p^3\ ^3D_1$
6	649.78	649.17	−2.135	153 898	153 898	$4s^24p5p\ ^3D_2$–$4s4p^3\ ^3D_2$
9	629.00	629.47	−1.414	158 982	158 982	$4s^24p5p\ ^3D_3$–$4s4p^3\ ^3D_3$
9	628.83	628.86	−1.018	159 025	159 025	$4s^24p5p\ ^3P_1$–$4s4p^3\ ^3D_1$
8	627.40	627.53	−2.219	159 388	159 380	$4s^24p5p\ ^1S_0$–$4s4p^3\ ^3P_1$
40wul	624.53	625.20	−0.664	160 120	160 122	$4s^24p5p\ ^3P_2$–$4s4p^3\ ^3D_3$
3	624.13	623.88	-2.660^b	160 223	160 219	$4s^24p5p\ ^3D_3$–$4s4p^3\ ^3D_2$
8	619.73	619.68	−1.339	161 361	161 359	$4s^24p5p\ ^3P_2$–$4s4p^3\ ^3D_2$
5	619.31	619.60	−2.426	161 470	161 480	$4s^24p5p\ ^3P_2$–$4s4p^3\ ^3D_1$
(4	603.91	604.14	−1.368	165 588	165 584	$4s^24p5p\ ^1D_2$–$4s4p^3\ ^3D_3$

Table 1. (Continued.)

Int. and shape[a]	λ_{obs} (Å)	λ_{pred} (Å)	Log gf	σ_{obs} (cm^{-1})	σ_{cal} (cm^{-1})[c]	Transition
12ul	586.31	585.90	−1.519	170 555	170 556	$4s^24p^2\,{}^1D_2$–$4s^24p4d\,{}^3F_2$
10	577.28	577.75	−2.109	173 226	173 226	$4s^24p^2\,{}^1D_2$–$4s^24p4d\,{}^3F_3$
9	547.38	547.08	−1.822	182 688	182 684	$4s^24p^2\,{}^3P_2$–$4s^24p4d\,{}^3F_2$
11w	539.50	539.97	−1.210	185 357	185 354	$4s^24p^2\,{}^3P_2$–$4s^24p4d\,{}^3F_3$
11ul	536.08	535.91	−1.854	186 539	186 536	$4s^24p^2\,{}^3P_1$–$4s^24p4d\,{}^3F_2$
7	495.72	495.82	0.019	201 727	201 722	$4s^24p^2\,{}^1S_0$–$4s^24p5s\,{}^3P_1$
7	472.19	472.22	0.037	211 779	211 789	$4s^24p^2\,{}^1S_0$–$4s^24p5s\,{}^1P_1$
5	452.08	452.03	−2.672[b]	221 200	221 203	$4s^24p^2\,{}^1D_2$–$4s^24p5s\,{}^3P_1$
6	440.37	440.29	−1.168	227 082	227 075	$4s^24p^2\,{}^1D_2$–$4s^24p5s\,{}^3P_2$
15	432.41	432.33	0.034	231 262	231 270	$4s^24p^2\,{}^1D_2$–$4s^24p5s\,{}^1P_1$
12d	428.56	428.57	−0.679	233 340	233 331	$4s^24p^2\,{}^3P_2$–$4s^24p5s\,{}^3P_1$
10	421.63	421.68	−0.855	237 175	237 183	$4s^24p^2\,{}^3P_1$–$4s^24p5s\,{}^3P_1$
15w	418.08	418.01	−0.109	239 234	239 203	$4s^24p^2\,{}^3P_2$–$4s^24p5s\,{}^3P_2$
10	415.08	415.13	−0.692	240 917	240 926	$4s^24p^2\,{}^3P_0$–$4s^24p5s\,{}^3P_1$
10	411.45	411.45	−0.519	243 043	243 055	$4s^24p^2\,{}^3P_1$–$4s^24p5s\,{}^3P_2$
6	410.87	410.83	−1.658[b]	243 386	243 398	$4s^24p^2\,{}^3P_2$–$4s^24p5s\,{}^1P_1$
6	404.45	404.49	−1.761	247 249	247 250	$4s^24p^2\,{}^3P_1$–$4s^24p5s\,{}^1P_1$

[a] Lines with cancellation factor (Cowan 1981) <0.05.

[b] Calculated wavenumber.

Table 2. New energy levels of the $4s^24p4d$, $4s^24p5s$ and $4s^24p5p$ configurations of Kr v.

Designation		E_{exp} (cm^{-1})	E_{calc} (cm^{-1})[a]	Percentage composition[b]
$4s^24p4d$	${}^3F_2$	190 279	190 362	99
	${}^3F_3$	192 949	192 770	99
	${}^3F_4$	—	196 425	100
$4s^24p5s$	${}^3P_0$		238 871	99
	${}^3P_1$	240 926	240 908	67 + 24 $4s^24p4d\,{}^1P$ + 5 $4s4p^3\,{}^1P$
	${}^3P_2$	246 798	246 806	100
	${}^1P_1$	250 993	250 987	79 + 12 $4s^24p5s\,{}^3P$ + 7 $4s^24p4d\,{}^1P$
$4s^24p5p$	${}^3D_1$	278 928	278 926	56 + 42 $4s^24p5p\,{}^1P$
	${}^3D_2$	283 677	283 745	85 + 8 $4s^24p5p\,{}^3P$ + 6 $4s^24p5p\,{}^1D$
	${}^3D_3$	289 998	289 992	99
	${}^3P_0$	—	284 942	92 + 6 $4s^24p5p\,{}^1S$
	${}^3P_1$	288 683	288 722	64 + 22 $4s^24p5p\,{}^1P$ + 12 $4s^24p5p\,{}^3D$
	${}^3P_2$	291 138	291 079	78 + 13 $4s^24p5p\,{}^3D$ + 8 $4s^24p5p\,{}^1D$
	${}^3S_1$	293 705	293 699	86 + 9 $4s^24p5p\,{}^3P$
	${}^1D_2$	296 600	296 656	85 + 13 $4s^24p5p\,{}^3P$
	${}^1P_1$	283 559	283 488	32 + 32 $4s^24p5p\,{}^3D$ + 26 $4s^24p5p\,{}^3P$ + 9 $4s^24p5p\,{}^3S$
	${}^1S_0$	307 667	307 640	68 + 21 $4p^4\,{}^1S$

[a] Calculated energy level values obtained using the fitted energy parameters.

[b] Percentages below 5% have been omitted.

results in the least-squares fit. The standard deviation was 124 cm^{-1}. If we compare this work with the report of Trigueiros *et al* (1989), we find that our electrostatic energy parameters are lower than those reported in that paper, except for the $G^3(4p4d)$ parameter of the $4s^24p4d$

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

Configuration	Parameter	HF value	Fitted value	F/HF
$4s4p^3$	E_{av}	148 381	151 658 ± 63	1.022 ± 0.001
	$F^2(4p, 4p)$	65 943	48 764 ± 493	0.739 ± 0.007
	$\alpha(4p, 4p)$		−659 (FIX)	
	ζ_{4p}	4619	5949 ± 106	1.287 ± 0.023
	$G^1(4s,4p)$	88 242	64 666 ± 181	0.733 ± 0.002
$4s^24p4d$	E_{av}	208 466	206 922 ± 52	0.993 ± 0.001
	ζ_{4p}	4784	4528 ± 109	0.946 ± 0.023
	ζ_{4d}	273	273 (FIX)	1.000
	$F^2(4p,4d)$	52 205	41 807 ± 426	0.801 ± 0.008
	$G^1(4p, 4d)$	62 999	48 954 ± 204	0.777 ± 0.003
	$G^3(4p, 4d)$	39 020	29 318 ± 485	0.751 ± 0.012
$4s^24p5s$	E_{av}	245 727	245 132 ± 97	0.998 ± 0.001
	ζ_{4p}	4953	5309 ± 182	1.172 ± 0.036
	$G^1(4p, 5s)$	7504	6283 ± 306	0.837 ± 0.041
Configuration interaction integrals				
$4s4p^3$–$4s^24p4d$	$R^1(4p4p, 4s4d)$	72 645	57 252 (FIX)	0.788
$4s4p^3$–$4s^24p5s$	$R^1(4p4p, 4s5s)$	1472	1252 (FIX)	0.850
$4s^24p4d$–$4s^24p5s$	$R^2(4p4d, 4p5s)$	−10 756	−9143 (FIX)	0.850
	R^1 (4p4d, 5s4p)	−3103	−2638 (FIX)	0.850

configuration. The inclusion of the $^3F_2$ and $^3F_3$ levels of the $4s^24p4d$ configuration and the three new energy levels of the $4s^24p5s$ configuration affect this calculation, although the interaction integrals with the latter are not very significant.

For the even parity the matrix included the $4s^24p^2 + 4s^24p5p + 4s4p^24d + 4p^4 + 4s^24p4f$ configurations. The configuration interaction integrals among these configurations are very strong except for those involving the $4s^24p5p$ because this has little influence on the calculation. The fitted average energy value of the $4s^24p^2$ configuration is affected when we include the $4p^4$ and $4s4p^24d$ configurations in the calculation. The fitted value is increased by 8022.74 cm^{-1} with respect to the experimental energy value. If we consider in the calculation only the $4s^24p^2 + 4s^24p5p$ configurations, the average energy value maintains its real value but the standard deviation increases substantially.

The levels belonging to the $4s4p^24d$ configuration are intermixed with the levels of the $4p^4$ configuration. For this reason we did not fix E_{av} for both configurations in the least-squares fit calculation. The energy parameters ζ_{nl}, $F^k(nl, nl)$ and $G^k(nl, nl)$ for the $4s4p^24d$ configuration were fixed at 1.00, 0.85 and 0.85 of their Hartree–Fock values respectively.

From the $4s^24p^2$ and $4p^4$ we obtained two adjusted parameters (in addition to E_{av}), by linking together all Coulomb parameters $F_2(4p4p)$ in one group and the spin–orbit parameter ζ_{4p} in a second group. A similar procedure was adopted in the work of Cavalcanti *et al* (1996) for Ar v. These authors also include ns^2nd^2 ($n = 3$) type configurations in the calculation, but in our case ($n = 4$) this was not necessary because the E_{av} is so far from the other configurations. However, we included the same ns^2np4f ($n = 4$) type configurations as Gallardo *et al* (1999) for Xe v ($n = 5$), as this reduces the standard deviation in our calculation. The energy parameters E_{av}, ζ_{nl}, $F^k(nl, nl)$ and $G^k(nl, nl)$ for the ns^2np4f configuration were fixed at 1.00, 1.00, 0.85 and 0.85 of their Hartree–Fock values respectively.

All the configuration interaction integrals were held fixed in the calculation at 0.85 of their Hartree–Fock values, except for the direct radial integrals of the $4s^24p^2$–$4p^4$, $4s4p^24d$–$4p^4$ and $4s4p^24d$–$4s^24p4f$ that were fixed in the calculation to 0.75, 0.70 and 0.75 of their Hartree–Fock

Table 4. Energy parameters (cm^{-1}) for the even-parity configurations of Kr v studied. (Note: the values for the E_{av} listed in the column 'HF value' were obtained by adding the experimental average energy of the ground configuration to the Hartree–Fock values.)

Configuration	Parameter	HF value	Fitted value	F/HF
$4s^24p^2$	E_{av}	12 468	20 491 ± 43	1.643 ± 0.003
	$F^2(4p, 4p)$	65 984[a]	52 183 ± 216	0.791 ± 0.003
	$\alpha(4p, 4p)$		90 (FIX)	
	ζ_{4p}	4627[a]	5008 ± 64	1.082 ± 0.014
$4s^24p5p$	E_{av}	289 834	289 398 ± 31	0.998 ± 0.001
	ζ_{4p}	5014	5 379 ± 72	1.073 ± 0.014
	ζ_{5p}	1255	1 420 ± 69	1.131 ± 0.055
	$F^2(4p, 5p)$	21 614	19 865 ± 303	0.919 ± 0.014
	$G^0(4p, 5p)$	5302	4 036 ± 57	0.761 ± 0.011
	$G^2(4p, 5p)$	6671	4 961 ± 332	0.744 ± 0.050
$4p^4$	E_{av}	309959	291 684 ± 997	0.941 ± 0.003
	$F^2(4p, 4p)$	65 920[a]	443 212 ± 184	0.672 ± 0.003
	$\alpha(4p, 4p)$		0 (FIX)	
	ζ_{4p}	4616[a]	4 995 ± 63	1.082 ± 0.013
$4s4p^24d$	E_{av}	335 994	333 337 ± 398	0.992 ± 0.001
	$F^2(4p, 4p)$	66 699	56 694 (FIX)	0.85
	$\alpha(4p, 4p)$		0 (FIX)	
	ζ_{4p}	4769	4769 (FIX)	1.000
	ζ_{4d}	282	282	1.000
	$F^2(4p, 4d)$	52 804	44 884 (FIX)	0.850
	$G^1(4s, 4p)$	89 160	75 786 (FIX)	0.850
	$G^2(4s, 4d)$	44 464	37 795 (FIX)	0.850
	$G^1(4p, 4d)$	64 061	54 452 (FIX)	0.850
	$G^3(4p, 4d)$	39 678	33 726 (FIX)	0.850
$4s^24p4f$	E_{av}	341 257	341 257 (FIX)	1.000
	ζ_{4p}	4986	4986 (FIX)	1.000
	ζ_{4f}	3	3 (FIX)	1.000
	$F^2(4p, 4f)$	27 406	23 295(FIX)	0.850
	$G^2(4p, 4f)$	18 274	15 533 (FIX)	0.850
	$G^4(4p, 4f)$	12 165	10 339 (FIX)	0.850
Configuration interaction integrals				
$4s^24p^2$–$4s^24p5p$	$R^0(4p4p, 4p5p)$	2325	1976 (FIX)	0.850
	$R^2(4p4p, 4p5p)$	10 824	9200 (FIX)	0.850
$4s^24p^2$–$4p^4$	$R^1(4s4s, 4p4p)$	88 211	66 159 (FIX)	0.750
$4s^24p^2$–$4s4p^24d$	$R^1(4s4p, 4p4d)$	73 683	62 631 (FIX)	0.850
	$R^2(4s4p, 4d4p)$	54 405	46 245 (FIX)	0.850
$4s^24p^2$–$4s^24p4f$	$R^2(4p4p, 4p4f)$	32 895	27 961 (FIX)	0.850
$4s^24p5p$–$4s4p^24d$	$R^1(4s5p, 4p4d)$	−2359	−2005 (FIX)	0.850
	$R^2(4s5p, 4d4p)$	7837	6662 (FIX)	0.850
$4s^24p5p$–$4s^24p4f$	$R^2(4p5p, 4p4f)$	−9187	−7809 (FIX)	0.850
	$R^2(4p5p, 4p4f)$	2381	2025 (FIX)	0.850
$4p^4$–$4s4p^24d$	$R^1(4p4p, 4s4d)$	73 265	51 285 (FIX)	0.700
$4s4p^24d$–$4s^24p4f$	$R^1(4p4d, 4s4f)$	46 595	34 946 (FIX)	0.750
	$R^2(4p4d, 4f4s)$	27 418	23 306 (FIX)	0.850

[a] Linked parameters. These parameters were linked (i.e. the mutual ratios of their values remained constant during the iteration) during the least-squares calculation (Cowan 1981).

values respectively. In this way we achieved better results in the least-squares fit. The standard deviation was 82 cm^{-1}.

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