



PREDICTED ENERGY LEVELS OF THE $4s4p4f$ AND $4p^24d$ CONFIGURATIONS OF THE FIVE TIMES IONIZED KRYPTON: Kr VI

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Abstract: The present study of the five times ionized krypton provides the predicted energy levels of the $4p^24d$ and $4s4p4f$ configurations. Theoretically, this study was supported with the pseudo-relativistic Hartree-Fock (HFR) method with the superposition of configuration interactions implemented in Cowan's suite of codes. For the first time, the 20 and 22 energy levels of the $4s4p4f$ and $4p^24d$ configurations, respectively, have been predicted.

Index Terms – Krypton, Kr-VI, Energy levels, Cowan code, Slater's parameters.

I. Introduction

Krypton is a chemically inert gas. Its atoms and ions are found in the Earth's atmosphere, liquid air, and cosmic objects, such as the hot Do-type white dwarf (RE0503-289)[1,2], planetary nebulae NGC7027 and NGC2440[3]. In recent investigations of the spectra of the hot Do-type white dwarfs, astronomers have observed 14 transitions of five time-ionized krypton (Kr VI) in the ultraviolet region (UV) of the spectrum[1,2]. Accurate atomic data (such as energy levels, transition rates, oscillator strengths, etc) of rare gas atoms and ions is important in various fields of physics, such as astrophysics, plasma physics, collision physics, laser physics, and photoelectron spectroscopy. In astrophysics, atomic data are useful in element abundance analysis inside cosmic objects and in understanding the energy transport mechanism through stars[4]. In plasma physics, atomic data are essential in determining the temperature[5,6] and concentrations of various plasma components[7]. In developing future ITER (International Thermonuclear Experimental Reactor) tokamak machines, the damage to plasma-facing components caused by excessive heat load is a major problem[8,9]. This problem could be mitigated by creating a peripheral radiating mantle that spreads the heat load and cools the outermost plasma region. For this purpose, the krypton gas is injected into the Tokamak machine.

The five-time ionized krypton is a member of the gallium (Ga) isoelectronic sequence and has a ground $4s^24p$ configuration, with two energy levels $^2P^{\circ}_{1/2}$, and $^2P^{\circ}_{3/2}$. The level $^2P^{\circ}_{1/2}$ represent the ground state energy level of Kr VI. For the first time, the spectrum of Kr VI was studied by Fawcett et.al[10], using a 3-meternormal incidence vacuum spectrograph, which had a reciprocal linear dispersion of $2.78\text{\AA}/\text{mm}$. The study used to photograph the ZETA spectrum was obtained for a discharge in deuterium (ZETA is a copious source of spectral lines emitted by highly ionized atoms in the vacuum ultraviolet). They reported the resonance transition arrays $4s^24p-4s4p^2$, and $4s^24p-4s^24d$ in the wavelength region of (400-1000) $\text{\AA}$ with an uncertainty of 0.03 $\text{\AA}$. In a subsequent study, Druetta et.al[11] reported three new lines belonging to the transition $4s^24p-4s4p^2$ array,

using the beam-foil technique. This study produced spectra in the wavelength region of (400-800) Å. In 1976, Livingston[12] reported four prominent transitions connecting the low-lying energy levels of Kr VI. The spectra were obtained using a beam-foil experiment conducted for lifetime comparison. In the study conducted by Reader et.al[13], the transition array between the configurations $4s^24p$ and $4s4p^2$ in gallium-like ions, specifically from Rb VII to In XIX, was observed and analyzed. Additionally, Trigueiros et.al[14] had reported seven new lines out of fifteen lines belonging to the $4s^24p$, $4s^25p$, $4s4p^2$, and $4s^24d$ configurations. These spectrograms were recorded using the theta pinch light source in the wavelength (450-1000)Å region with an estimated uncertainty of 0.01Å on a 3-m normal-incidence spectrograph. In a separate study, A Tauheed et.al [15] had identified the inter-combination lines connecting the $4s4p^2\ ^4P$, $4s^24p\ ^2P^o$ terms and also reported the lifetime for the $4s4p^2\ (^4P_{1/2},\ ^4P_{5/2})$, and $4p^3\ (^2D^o_{3/2},\ ^2D^o_{5/2})$ levels utilizing beam-foil spectra photographed in the range of 890 to 1010 Å. Following this, Pagan et.al[16] confirmed previous findings and reported 141 lines that established 44 energy levels. Subsequently, Pagan et.al[17] updated the previously observed wavelength data, along with their weighted oscillator strengths for all known electric dipole transitions of Kr VI. Furthermore, Sugar and Musgrove[18] had compiled the energy level data of references[14,15], and the wavelength data of references [14–16,19] was compiled by the T Shirai et.al[20]. All these updates (energy level and wavelength) were included in the compilation of Krypton and its ions (Kr I-XXXVI) by [21]. In 2011, Farias et.al[22] partially studied the $4s4p5p$, $4p^24d$, and $4s4p4f$ configurations. But the most of the levels of the $4s4p4f$ and $4p^24d$ configurations are still unknown. This motivates us to predict these unknown energy levels of the $4s4p4f$ and $4p^24d$ configurations.

II. Results and discussion

The theoretical calculations were performed using a pseudo-relativistic Hartree–Fock (HFR) method with a superposition of interacting configurations. These calculations were carried out using Cowan's suite of codes[23]. We used the Windows-based version of the Cowan codes, developed by A Kramida at NIST, Gaithersburg, available through the NIST website[24]. The configurations given in the Table (1) are incorporated in the relativistic Hartree-Fock calculations. In our calculation, the Slater's parameters were kept at 85% of the HFR value for F^k , 75% for G_k , 75% for the R^k , and the E_{av} and ζ_{nl} were fixed at 100% of their HFR values. Least-squares fitting (LSF) method was used to minimize the differences between the calculated and observed energy levels of Kr VI. The accuracy of the fit can be judged by standard deviation, which is calculated by the formula as given by the equation (16.1) in the book of R D Cowan [23]. The LSF method helps us verify the experimental energy levels and predict unknown energy levels. For the LSF calculations, we include all the energy levels reported by Pagan et.al[16] ,and Farias et.al[22] on the Kr VI ion. The LSF calculations were performed using the RCE20 code from the Cowan package. In both LSF calculations, the parameter-linking approach is employed, and some parameters were kept fixed for better fitting and a low standard deviation of fit. The standard deviation of the fit (SD) is given in Table (1) together with the total number of known energy levels and free parameters used in the fit, shown in curly brackets.

Farias et al [22] reported the two and six levels of the $4s4p4f$, and $4p^24d$ configurations, but the most of the levels of these configurations are still unknown. In this study, we have predicted the remaining unknown levels of these configurations for the first time using the least squares calculations (LSF), in which all the known levels of the Kr VI spectrum, are incorporated for predicting the unknown energy levels of the configurations. This method provides approximate energy levels values for the unknown energy levels, which are very useful for establishing the experimental energy levels. The predicted energy levels of the $4s4p4f$ and $4p^24d$ configurations along with their LS composition are given in the Table (2).

Table 1. The set of the interacting configurations used in the HFR calculation.

Odd parity	Even parity
4s ² nl (n= 10,l=p, f, n= 8,l=h)	4s4p ²
4p ² nl (n= 10,l=p, f, n= 8,l=h)	4s ² nl (n= 10, l=s)
4s4pnl (n= 7,l=s, d),4s4d(4,5)f	4s ² nl (n= 10, l=d)
4p4d ² ,4p4f ² ,4p5s ² ,4p5p ² ,4d ² 4f	4s4pnl (n= 8,l=p)
4p4d5s,4p4d5d,4d4f5s,4d4f5d	4s4pnl (n= 6,l=f)
4s5s5p,4s5s5f,4s4f5s,4s4f5d	4p ² nl (n= 10,l=s, d)
4s4d5p 4p ³ ,4d ² 5p,4f ² 5p	4s4d ² ,4s4f ² ,4s4d5s
.....	
No. of levels ^a = 33{17}	No. of levels ^a = 37{17}
SD = 247 cm ⁻¹	SD = 741 cm ⁻¹

^a Total number of known levels and free parameters in the LS fitting, the latter is given in the parentheses. SD→ Standard deviation of the LSF calculation.

Table 2. The predicted energy levels of the 4s4p4f and 4p²4d configurations of Kr VI.

E _{Predicted} , (kcm ⁻¹)	J	First % LS component	Second % LS component
458.5308	2.5 65	4s.4p.(3P*).4f 2F 23	4p2.(3P).4d 2F
460.1302	3.5 63	4s.4p.(3P*).4f 2F 19	4p2.(3P).4d 2F
460.7758	2.5 61	4s.4p.(3P*).4f 4F 32	4p2.(3P).4d 4F
463.251	4.5 68	4s.4p.(3P*).4f 4F 28	4p2.(3P).4d 4F
471.4757	3.5 47	4s.4p.(3P*).4f 2G 24	4s.4p.(3P*).4f 4G
471.6779	2.5 96	4s.4p.(3P*).4f 4G	
472.9909	3.5 59	4s.4p.(3P*).4f 4D 22	4p2.(3P).4d 4D
473.4004	2.5 61	4s.4p.(3P*).4f 4D 31	4p2.(3P).4d 4D
473.7038	1.5 59	4s.4p.(3P*).4f 4D 37	4p2.(3P).4d 4D
473.7052	3.5 71	4s.4p.(3P*).4f 4G 16	4s.4p.(3P*).4f 2G
473.8891	0.5 58	4s.4p.(3P*).4f 4D 40	4p2.(3P).4d 4D
474.1644	4.5 52	4s.4p.(3P*).4f 4G 33	4s.4p.(3P*).4f 2G
475.9806	4.5 45	4s.4p.(3P*).4f 4G 34	4s.4p.(3P*).4f 2G
477.1883	5.5 100	4s.4p.(3P*).4f 4G	
477.3133	2.5 75	4s.4p.(3P*).4f 2D 10	4p2.(3P).4d 2D
480.0131	1.5 76	4s.4p.(3P*).4f 2D 11	4p2.(3P).4d 2D
486.4572	3.5 62	4p2.(1D).4d 2F 14	4s.4p.(3P*).4f 2F
487.7733	1.5 55	4p2.(3P).4d 4F 32	4s.4p.(3P*).4f 4F
488.6452	2.5 59	4p2.(3P).4d 4F 31	4s.4p.(3P*).4f 4F
490.3641	0.5 64	4p2.(3P).4d 2P 22	4p2.(1D).4d 2P
492.9883	4.5 67	4p2.(3P).4d 4F 28	4s.4p.(3P*).4f 4F
496.4618	1.5 57	4p2.(3P).4d 4D 35	4s.4p.(3P*).4f 4D
496.5989	2.5 55	4p2.(3P).4d 4D 30	4s.4p.(3P*).4f 4D
496.8989	0.5 55	4p2.(3P).4d 4D 35	4s.4p.(3P*).4f 4D
505.7831	1.5 89	4p2.(3P).4d 4P 2	4p2.(1D).4d 2D
506.6276	0.5 96	4p2.(3P).4d 4P	
512.7968	1.5 67	4p2.(1D).4d 2D 9	4s.4d2.(1D) 2D
513.0434	2.5 64	4p2.(1D).4d 2D 9	4s.4d2.(1D) 2D
518.3085	1.5 43	4p2.(1S).4d 2D 29	4s.4p.(1P*).4f 2D
520.7288	2.5 28	4p2.(1S).4d 2D 27	4s.4p.(1P*).4f 2D
521.2214	3.5 75	4s.4p.(1P*).4f 2F 18	4p2.(3P).4d 2F
521.2925	2.5 50	4s.4p.(1P*).4f 2F 16	4s.4p.(1P*).4f 2D
521.4656	0.5 46	4p2.(1D).4d 2P 26	4p2.(3P).4d 2P

524.0868	1.5	41	4p2.(1D).4d	2P	25	4p2.(3P).4d	2P
527.7477	0.5	84	4p2.(1D).4d	2S	11	4s.4d2.(1S)	2S
533.8801	1.5	48	4p2.(3P).4d	2D	35	4s.4p.(1P*).4f	2D
533.9574	3.5	60	4s.4p.(1P*).4f	2G	19	4s.4d2.(1G)	2G
535.2428	2.5	42	4p2.(3P).4d	2D	15	4p2.(3P).4d	2F
535.641	4.5	61	4s.4p.(1P*).4f	2G	19	4s.4d2.(1G)	2G
537.9358	2.5	27	4p2.(3P).4d	2F	15	4p2.(3P).4d	2D
539.0384	3.5	44	4p2.(3P).4d	2F	16	4s.4d2.(3F)	2F
560.991	2.5	28	4p2.(1S).4d	2D	18	4s.4p.(1P*).4f	2D

III.Conclusion

In this work, we have used the Cowan suite of codes for predicting the unknown energy levels of Kr VI. The energy levels values of all the remaining unknown energy levels of the 4s4p4f, and 4p²4d configurations are predicted.

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