

A Collisional-Radiative Model for Kr III Ions

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Abstract: A collisional radiative model for Kr III in the ultraviolet regime is developed. For this purpose, atomic parameters for $4s^24p^4$, $4s4p^5$, $4s^24p^3nl$, and $4s^24p^35d$ configurations with n ranging from 5 to 7 and $l = s, p$, using the multiconfiguration Dirac–Hartree–Fock method are calculated. The effects of Breit and radiative quantum electrodynamic corrections are also included. Electron impact excitation cross-sections from the ground state, along with four metastable states arising from the $4s^24p^4$ configuration to all fine structure levels of interest, are calculated using the relativistic distorted wave method. The reliability of the model is tested by comparing the predicted results with the previous measurements.

Keywords: electron impact excitation; collision rate coefficients; Kr III; CR modelling

1. Introduction

Low-temperature krypton plasmas are present in diverse astrophysical and laboratory settings, and their examination holds significance for numerous technological plasma applications. Krypton is a cosmically abundant neutron (n)-capture element, with its various ionization states identified in more than 100 planetary nebulae in the Milky Way and nearby galaxies [1–3].

Further, Kr has been proven to be an ideal candidate for use as an impurity ion in fusion plasma diagnosis and modeling [4,5]. In the high temperature of the fusion plasma, lower Z impurities, like nitrogen and argon, become unsuitable. Instead, higher Z impurities, such as Kr and Xe, are necessary to interpret plasma line emissions accurately [6,7]. Therefore, spectroscopic studies, especially of the first few initial ionization states of Kr, are of critical importance. Due to the extensive emission spectra of krypton, its ions are particularly interesting for producing light sources and lamps, and for developing lasers and laser techniques [8]. Additionally, Kr and other inert gases are used as trace gases and are introduced to characterize low-temperature plasmas. Efficient modeling of krypton-containing plasmas, therefore, holds significant implications for optimizing these technologies and advancing their capabilities [9–11]. Moreover, Kr can serve as an alternative propellant to xenon for use in electrostatic spacecraft propulsion thrusters [12,13]. Developing electric propulsion systems involves complex plasma physics and secondary effects, necessitating thorough testing and study for flight qualification. To address this, an effective plasma diagnosis approach is required. In addition to Kr-lines, the lines from its ions, like Kr II–III, can also be emitted in the Kr-thruster and other laboratory and astrophysical plasma. Developing a suitable collisional radiative (CR) model for these ions is equally important, as it can also be utilized for diagnostics.

Conventional methods for plasma diagnosis typically involve probe measurements. However, these approaches are deemed unsuitable due to their disruptive nature on plasma conditions. Therefore, non-intrusive diagnostic methods like optical emission spectroscopy (OES) are preferred. The development of a quantitative OES diagnostic predominantly relies on constructing a collisional radiative model to interpret plasma parameters, e.g., electron temperature and densities, from plasma line emission intensities.



Citation: Rathī, S.; Sharma, L. A Collisional-Radiative Model for Kr III Ions. *Atoms* **2024**, *12*, 39. <https://doi.org/10.3390/atoms12080039>

Received: 14 June 2024

Revised: 15 July 2024

Accepted: 23 July 2024

Published: 29 July 2024



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Various studies have been carried out in the past to study low-temperature Kr plasma. Zhu et al. [14], investigated the electron energy distribution in capacitively coupled and inductively coupled argon and krypton plasmas by analyzing emission line ratios. They presented a comprehensive CR model, which, in combination with a set of emission line ratios of argon and krypton, was employed to ascertain the electron energy distribution function characterized by a “two-temperature” structure in low-pressure plasma. Later, a detailed collisional radiative model for Kr was developed by Gangwar et al. [15]. They applied the model for the characterization of inductively coupled Kr plasma. Other studies include a detailed collisional radiative model for Kr II by Agrawal et al. [16]. Further, for low-temperature plasma diagnosis, electron impact excitation (EIE) cross-sections are crucial. Therefore, many studies in the past have focused on the calculation of these parameters [4,10,17]. However, these studies are limited to Kr and Kr II. For Kr III, to the best of our knowledge, we found no detailed work either for the electron impact excitation cross-sections or for a CR model. The development of CR models tailored for Kr III is essential for understanding and characterizing the plasma behavior.

Thus, in light of the above discussion, the objective of this study is to construct a detailed collisional radiative model for a low-temperature Kr III plasma. The main challenge in creating a reliable CR model arises from the necessity for accurate and comprehensive atomic data. In addition to level energies and radiative transition rates (A), electron-induced processes, specifically electron impact excitation of various fine-structure transitions, play a crucial role. To address this issue, we performed a detailed spectroscopic analysis of Kr III and calculated the energies and transition rates for transition among $4s^2 4p^4$, $4s 4p^5$, $4s^2 4p^3 4d$, $4s^2 4p^3 5d$, $4s^2 4p^3 6d$, and $4s^2 4p^3 nl$ configurations, where n ranges from 5 to 7 with $l = s$ and p . The bound state wave functions for the considered levels were built in the framework of multiconfiguration Dirac–Hartree–Fock (MCDHF) [18] theory. The EIE cross-sections using the relativistic distorted wave (RDW) approximation [19] from the ground configuration to all the considered configurations were calculated for the incident electron with energies ranging from threshold to 300 eV.

The present model is validated by coupling it with the emission spectroscopy measurements of Belmonte et al. [8] and performing a diagnosis of the low-temperature Kr III plasma. They measured transition probabilities of 62 lines of Kr III in the 213–362 nm wavelength range using the low-pressure pulsed arc plasma technique. In this work, the plasma parameters, viz., electron density and temperature, are determined by analyzing the agreement between our CR model and experimental intensities [8], following a least deviation approach.

2. Theoretical Approach

2.1. MCDHF

The first step in building our CR model was to generate reliable bound state wavefunctions, which we used to calculate the atomic structure parameters and electron impact excitation cross-sections. The quality of the wavefunction can significantly influence the accuracy of the computed parameters. Therefore, we employed the fully relativistic MCDHF [20] approach implemented in the GRASP2018 [21]. For the present work, we chose five even configurations, $4s^2 4p^4$, $4p^6$, $4s^2 4p^3 5p$, $4s^2 4p^3 6p$, and $4s^2 4p^3 7p$, and seven odd configurations, $4s 4p^5$, $4s^2 4p^3 4d$, $4s^2 4p^3 5s$, $4s^2 4p^3 5d$, $4s^2 4p^3 6s$, $4s^2 4p^3 6d$, and $4s^2 4p^3 7s$. All these configurations together formed our multireference set. The ground state of Kr III, $4s^2 4p^4$, had four electrons in the p orbital, making it a complicated system due to a considerable amount of electron correlation effects and spin-orbit coupling. To account for this, configuration state functions (CSFs) were expanded up to $n = 9$ and $l = s, p, d$ orbitals. We limited the contribution of the f orbital to $n = 4$ and 5 shells only. The CSFs and mixing coefficients were then optimised using the relativistic self-consistent field approach. Further, the effects of Breit, vacuum polarization, and self-energy corrections were included in the relativistic configuration interaction (RCI) calculations.

2.2. RDW Approximation

We computed the electron impact excitation cross-sections in the relativistic distorted wave approximation framework using the above-obtained bound state wavefunctions. This method has shown promising results for a variety of targets, including neutral atoms and their low-and highly-charged states, as well as closed and open-shell systems [19,22,23]. A thorough comprehension of the theory can be obtained from our research group's prior works [19,24]. The T -matrix for an electron transitioning from an initial state r to a final state s can be expressed as follows using the RDW approximation:

$$T_{RDW}^{r \rightarrow s}(\gamma_s J_s M_s \mu_s; \gamma_r J_r M_r \mu_r) = \langle \zeta_s^- | V - U_D(N+1) | \mathcal{A} \zeta_r^+ \rangle. \quad (1)$$

Here, the total angular momentum quantum number and its magnetic quantum number are denoted by $J_{r(s)}$ and $M_{r(s)}$, respectively, while the additional quantum numbers and the spin projection of the arriving (scattered) electron are denoted by γ and $\mu_{r(s)}$, respectively. For the projectile electron and the target electrons, the exchange is explained by the antisymmetric operator $\mathcal{A}$. The distorted potential U_D is selected as a spherically averaged static potential from the excited state of the ion based on the projectile electron's radial coordinates. The Coulomb interaction between the target ion and the incoming electron is represented by the interaction potential V . The N -electron target's wavefunction in state $s(r)$ and the projectile electron's distorted wavefunction are multiplied to create the wavefunction $\zeta_{s(r)}^{-(+)}$, where symbols $-(+)$ denote an incoming (outgoing) wave. By squaring the modulus of Equation (1) and performing the necessary normalization, the integral cross-section is computed as follows:

$$\sigma_{r \rightarrow s} = (2\pi)^4 \frac{k_s}{k_r} \frac{1}{2(2J_r + 1)} \sum_{M_s \mu_s} \sum_{M_r \mu_r} \int |T_{RDW}^{r \rightarrow s}|^2 d\Omega. \quad (2)$$

Here, k_r and k_s denote the linear momenta of the incident and scattered electrons, respectively.

3. Results and Discussion

3.1. Energies and Transition Rates

To check the accuracy of the present wavefunctions, we compared the present calculated energies with the energies available from the National Institute of Standards and Technology, Atomic Spectra Database (NIST ASD) [25]. At NIST, energies of 123 levels of Kr III were compiled by Salmon [26]. The compilation of Salmon included the measurement of Bredice et al. [27], Almandos et al. [28], and Raineri et al. [29]. The two results are shown in Table 1. Clearly, our energies agreed well with the NIST data, with a root-mean-square deviation of 0.4667 eV.

Table 1. The present calculated energies (in eV) and their comparison with the NIST energy data.

Level	Energies (eV)		Level	Energies (eV)	
	NIST	Present		NIST	Present
$4s^2 4p^4 \ ^3P_2$	0	0	$4s^2 4p^3 ({}^2D) 5p \ ^3F_3$	24.03125	23.6193
$4s^2 4p^4 \ ^3P_1$	0.56393	0.5428	$4s^2 4p^3 ({}^2D) 5p \ ^3D_2$	24.035001	23.4991
$4s^2 4p^4 \ ^3P_0$	0.65872	0.6369	$4s^2 4p^3 ({}^2D) 5p \ ^1P_1$	24.067844	23.6501
$4s^2 4p^4 \ ^1D_2$	1.81566	1.9110	$4s^2 4p^3 ({}^2D) 5p \ ^1F_3$	24.172308	23.8821
$4s^2 4p^4 \ ^1S_0$	4.10135	3.9061	$4s^2 4p^3 ({}^2D) 5p \ ^3D_3$	24.236183	23.7685
$4s 4p^5 \ ^3P_2$	14.373603	13.7131	$4s^2 4p^3 ({}^2D) 5p \ ^3F_4$	24.260546	23.8377
$4s 4p^5 \ ^3P_1$	14.801262	14.1146	$4s^2 4p^3 ({}^2P) 4d \ ^1F_3$	24.336391	25.0925
$4s 4p^5 \ ^3P_0$	15.069406	14.3671	$4s^2 4p^3 ({}^2D) 5p \ ^3P_2$	24.562234	24.4161
$4s^2 4p^3 ({}^4S) 4d \ ^5D_0$	17.165202	16.3392	$4s^2 4p^3 ({}^2D) 5p \ ^3P_0$	24.646677	24.4735
$4s^2 4p^3 ({}^4S) 4d \ ^5D_1$	17.168212	16.3402	$4s^2 4p^3 ({}^2D) 5p \ ^3P_1$	24.651078	24.4653

Table 1. Cont.

Level	Energies (eV)		Level	Energies (eV)	
	NIST	Present		NIST	Present
$4s^2 4p^3 ({}^4S) 4d {}^5D_2$	17.169406	16.3398	$4s^2 4p^3 ({}^2D) 5p {}^1D_2$	25.15589	25.0686
$4s^2 4p^3 ({}^4S) 4d {}^5D_3$	17.170888	16.3434	$4s^2 4p^3 ({}^2P) 5p {}^3D_1$	25.695354	25.5247
$4s^2 4p^3 ({}^4S) 4d {}^5D_4$	17.190304	16.3586	$4s^2 4p^3 ({}^2P) 5p {}^3D_2$	25.851944	25.661
$4s 4p^5 {}^1P_1$	17.590402	17.1945	$4s^2 4p^3 ({}^2P) 5p {}^3S_1$	25.864287	25.6377
$4s^2 4p^3 ({}^4S) 5s {}^5S_2$	18.066837	17.3267	$4s^2 4p^3 ({}^2P) 5p {}^3P_1$	25.94796	25.8534
$4s^2 4p^3 ({}^4S) 4d {}^3D_2$	18.325429	17.9033	$4s^2 4p^3 ({}^2P) 5p {}^3P_0$	26.010191	25.9622
$4s^2 4p^3 ({}^4S) 4d {}^3D_3$	18.440829	17.9794	$4s^2 4p^3 ({}^2P) 5p {}^3D_3$	26.020381	25.8194
$4s^2 4p^3 ({}^4S) 4d {}^3D_1$	18.482554	18.0286	$4s^2 4p^3 ({}^2P) 5p {}^1D_2$	26.299951	26.3276
$4s^2 4p^3 ({}^4S) 5s {}^3S_1$	18.793548	18.3347	$4s^2 4p^3 ({}^2P) 5p {}^1P_1$	26.31735	26.1997
$4s^2 4p^3 ({}^2D) 4d {}^3F_2$	19.03941	18.6926	$4s^2 4p^3 ({}^2P) 5p {}^3P_2$	26.415767	26.295
$4s^2 4p^3 ({}^2D) 4d {}^1S_0$	19.143124	18.9904	$4s^2 4p^3 ({}^4S) 6s {}^5S_2$	26.72122	25.758
$4s^2 4p^3 ({}^2D) 4d {}^3F_3$	19.180338	18.8405	$4s^2 4p^3 ({}^4S) 5d {}^5D_0$	26.842635	25.9435
$4s^2 4p^3 ({}^2D) 4d {}^3F_4$	19.351697	18.9913	$4s^2 4p^3 ({}^4S) 5d {}^5D_1$	26.844388	25.944
$4s^2 4p^3 ({}^2D) 4d {}^3G_3$	19.837029	19.5961	$4s^2 4p^3 ({}^4S) 5d {}^5D_2$	26.846142	25.9445
$4s^2 4p^3 ({}^2D) 4d {}^3G_4$	19.888908	19.6399	$4s^2 4p^3 ({}^4S) 5d {}^5D_3$	26.848131	25.945
$4s^2 4p^3 ({}^2D) 4d {}^3G_5$	19.974922	19.6921	$4s^2 4p^3 ({}^4S) 5d {}^5D_4$	26.855511	25.949
$4s^2 4p^3 ({}^2D) 4d {}^1G_4$	20.189717	20.0581	$4s^2 4p^3 ({}^4S) 6s {}^3S_1$	26.951175	26.0715
$4s^2 4p^3 ({}^2D) 5s {}^3D_1$	20.242766	20.0101	$4s^2 4p^3 ({}^4S) 5d {}^3D_2$	27.448687	26.8588
$4s^2 4p^3 ({}^2D) 5s {}^3D_2$	20.288258	20.0529	$4s^2 4p^3 ({}^4S) 5d {}^3D_3$	27.495681	26.881
$4s^2 4p^3 ({}^2D) 5s {}^3D_3$	20.46402	20.1883	$4s^2 4p^3 ({}^4S) 5d {}^3D_1$	27.49775	26.9104
$4s^2 4p^3 ({}^2P) 4d {}^1D_2$	20.514847	20.2645	$4s^2 4p^3 ({}^2D) 5d {}^3D_2$	28.902074	28.8061
$4s^2 4p^3 ({}^2D) 4d {}^1D_1$	21.102396	21.1161	$4s^2 4p^3 ({}^2D) 5d {}^1S_0$	28.905521	28.5747
$4s^2 4p^3 ({}^2D) 5s {}^1D_2$	21.188768	21.2353	$4s^2 4p^3 ({}^2D) 5d {}^3G_4$	28.91979	28.606
$4s^2 4p^3 ({}^2P) 4d {}^3P_0$	21.32477	21.304	$4s^2 4p^3 ({}^2D) 6s {}^3D_2$	28.931251	28.3947
$4s^2 4p^3 ({}^2D) 4d {}^3D_2$	21.382994	21.3741	$4s^2 4p^3 ({}^2D) 5d {}^3D_1$	29.014873	28.7654
$4s^2 4p^3 ({}^2P) 4d {}^3P_1$	21.447172	21.458	$4s^2 4p^3 ({}^2D) 5d {}^3D_3$	29.059434	28.8263
$4s^2 4p^3 ({}^2D) 4d {}^3D_3$	21.629161	21.6529	$4s^2 4p^3 ({}^2D) 6s {}^3D_3$	29.082588	28.5158
$4s^2 4p^3 ({}^2P) 4d {}^3F_3$	21.676239	21.6721	$4s^2 4p^3 ({}^2D) 6s {}^1D_2$	29.158831	28.636
$4s^2 4p^3 ({}^2P) 4d {}^3F_4$	21.702564	21.6694	$4s^2 4p^3 ({}^2D) 5d {}^3F_4$	29.180492	28.6806
$4s^2 4p^3 ({}^2P) 4d {}^3F_2$	21.723415	21.7447	$4s^2 4p^3 ({}^4S) 6d {}^5D_1$	29.18709	29.3112
$4s^2 4p^3 ({}^4S) 5p {}^5P_1$	21.76466	20.9086	$4s^2 4p^3 ({}^2D) 5d {}^1G_4$	29.262809	28.7683
$4s^2 4p^3 ({}^4S) 5p {}^5P_2$	21.793774	20.9397	$4s^2 4p^3 ({}^4S) 6d {}^5D_2$	29.282912	29.3084
$4s^2 4p^3 ({}^4S) 5p {}^5P_3$	21.885693	21.0073	$4s^2 4p^3 ({}^4S) 6d {}^5D_3$	29.321552	29.3128
$4s^2 4p^3 ({}^2P) 4d {}^3P_2$	21.919259	21.8438	$4s^2 4p^3 ({}^2D) 5d {}^3P_2$	29.40363	29.361
$4s^2 4p^3 ({}^2P) 5s {}^3P_0$	22.09938	22.1812	$4s^2 4p^3 ({}^2D) 5d {}^1P_1$	29.411375	29.5393
$4s^2 4p^3 ({}^2P) 5s {}^3P_1$	22.1013	22.2034	$4s^2 4p^3 ({}^2D) 5d {}^3P_0$	29.430526	29.3017
$4s^2 4p^3 ({}^4S) 5p {}^3P_1$	22.271137	21.627	$4s^2 4p^3 ({}^2D) 5d {}^3S_1$	29.504579	29.1699
$4s^2 4p^3 ({}^4S) 5p {}^3P_2$	22.32744	21.672	$4s^2 4p^3 ({}^2D) 5d {}^1D_2$	29.583614	29.4387
$4s^2 4p^3 ({}^4S) 5p {}^3P_0$	22.346555	21.6797	$4s^2 4p^3 ({}^4S) 6d {}^3D_3$	29.759332	29.8347
$4s^2 4p^3 ({}^2P) 5s {}^3P_2$	22.347791	22.4825	$4s^2 4p^3 ({}^2P) 5d {}^3F_2$	30.646034	30.5037
$4s^2 4p^3 ({}^2D) 4d {}^3S_1$	22.473805	22.771	$4s^2 4p^3 ({}^2P) 5d {}^3F_3$	30.648076	30.5708
$4s^2 4p^3 ({}^2P) 5s {}^1P_1$	22.597971	22.6612	$4s^2 4p^3 ({}^2P) 6d {}^3P_0$	30.862835	32.1173
$4s^2 4p^3 ({}^2D) 4d {}^1F_3$	22.684996	22.938	$4s^2 4p^3 ({}^2P) 6s {}^3P_1$	30.892804	30.3303
$4s^2 4p^3 ({}^2P) 4d {}^3D_3$	22.923664	23.2994	$4s^2 4p^3 ({}^2P) 6s {}^3P_2$	30.91693	30.5728
$4s^2 4p^3 ({}^2P) 4d {}^3D_2$	23.022456	23.5221	$4s^2 4p^3 ({}^2P) 5d {}^3P_1$	30.926328	30.9189
$4s^2 4p^3 ({}^2P) 4d {}^3D_1$	23.337946	23.7662	$4s^2 4p^3 ({}^2P) 6s {}^1P_1$	30.974683	30.681
$4s^2 4p^3 ({}^2D) 4d {}^3P_2$	23.379594	24.1609	$4s^2 4p^3 ({}^2P) 5d {}^3P_0$	31.071757	30.9028
$4s^2 4p^3 ({}^2D) 4d {}^3P_1$	23.585044	24.4554	$4s^2 4p^3 ({}^2P) 5d {}^1D_2$	31.10901	31.0026
$4s^2 4p^3 ({}^2D) 5p {}^3D_1$	23.64671	23.2735	$4s^2 4p^3 ({}^2P) 5d {}^1F_3$	31.24481	31.1903
$4s^2 4p^3 ({}^2D) 5p {}^3F_2$	23.891984	23.6566	$4s^2 4p^3 ({}^2D) 6d {}^3S_1$	31.971241	32.1922
$4s^2 4p^3 ({}^2D) 4d {}^1D_2$	24.009753	24.5708			

Further, we compared the present calculated transition rates with the rates provided by Belmonte et al. [8] in Figure 1. Almost all of the transition rates were within the same order of magnitude as the measurements of [8] with the majority of the data points clustered

around a ratio value of one. A good agreement of present energies and transition probabilities with the results of [8], and NIST aided us in establishing the fact that the present wavefunctions were generated properly enough to provide results with a good accuracy.

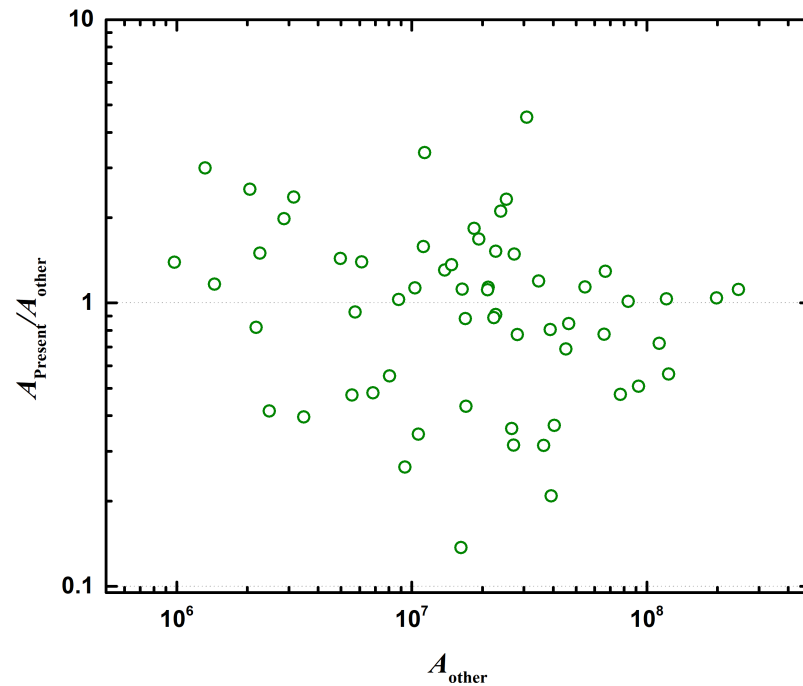


Figure 1. Comparison of the present transition rates (A_{Present}) with the measured transition rates (A_{Other}) of [8].

3.2. EIE Cross-Sections

We implemented the above-obtained bound state MCDHF wavefunctions to solve the T -matrix for an electron-induced transition as defined in Equation (1), and determined the EIE cross-section for the desired transitions using Equation (2). We compute the EIE cross-section for transitions from the ground ($4s^24p^4\ ^3P_2$) and four metastable states ($4s^24p^4\ ^3P_{1,0}$, $^1D_2$, $^1S_0$) to higher lying levels for an incident electron in the energy range from threshold to 300 eV. The lifetimes of these levels obtained from the present calculations were 0.58, 40.65, 0.17, and 0.02 s, respectively.

The calculated cross-sections for a few transitions are shown in Figures 2 and 3. Figure 2a,b show the EIE cross-sections for transitions from $4s^24p^4\ ^3P_2$ and $4s^24p^4\ ^3P_0$ states to the fine structure levels of $4s^24p^4$ and $4s4p^5$ configurations. Clearly, the probability of an electric dipole transition from $4s^24p^4\ ^3P_{2,0}$ to $4s4p^5$ was higher compared with forbidden transitions among the fine structure levels of $4s^24p^4$. This pattern was in agreement with the general behaviour of EIE cross-sections. Moreover, we show EIE cross-sections for the transition from $4s^24p^4\ ^3P_2$ to various fine structure levels of $4s^24p^34d$ and $4s^24p^35p$ in Figure 3. For brevity, we present only a few cross-section results here. We found no previous measurement or calculation to compare our EIE cross-sections. Moreover, using these computed cross-sections, we calculated the rate coefficients in the temperature range of 0–50 eV by considering a Maxwellian electron energy distribution function. The expression for rate coefficients is as follows:

$$R_{r \rightarrow s} = 2 \left(\frac{2}{\pi m_e} \right)^{1/2} (k_B T)^{-3/2} \int_{E_{rs}}^{\infty} E \sigma_{r \rightarrow s}(E) \exp\left(\frac{-E}{k_B T}\right) dE. \quad (3)$$

Here, the threshold energy of transition $r \rightarrow s$ is given by E_{rs} . The Boltzmann constant and the mass of an electron are represented by the symbols k_B and m_e , respectively.

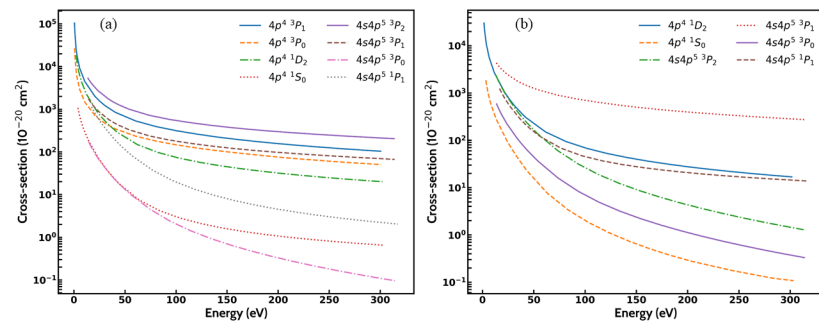


Figure 2. EIE cross-sections for transitions from the (a) $4s^2 4p^4 \ ^3P_2$ and (b) $4s^2 4p^4 \ ^3P_0$, levels of Kr III to higher excited levels.

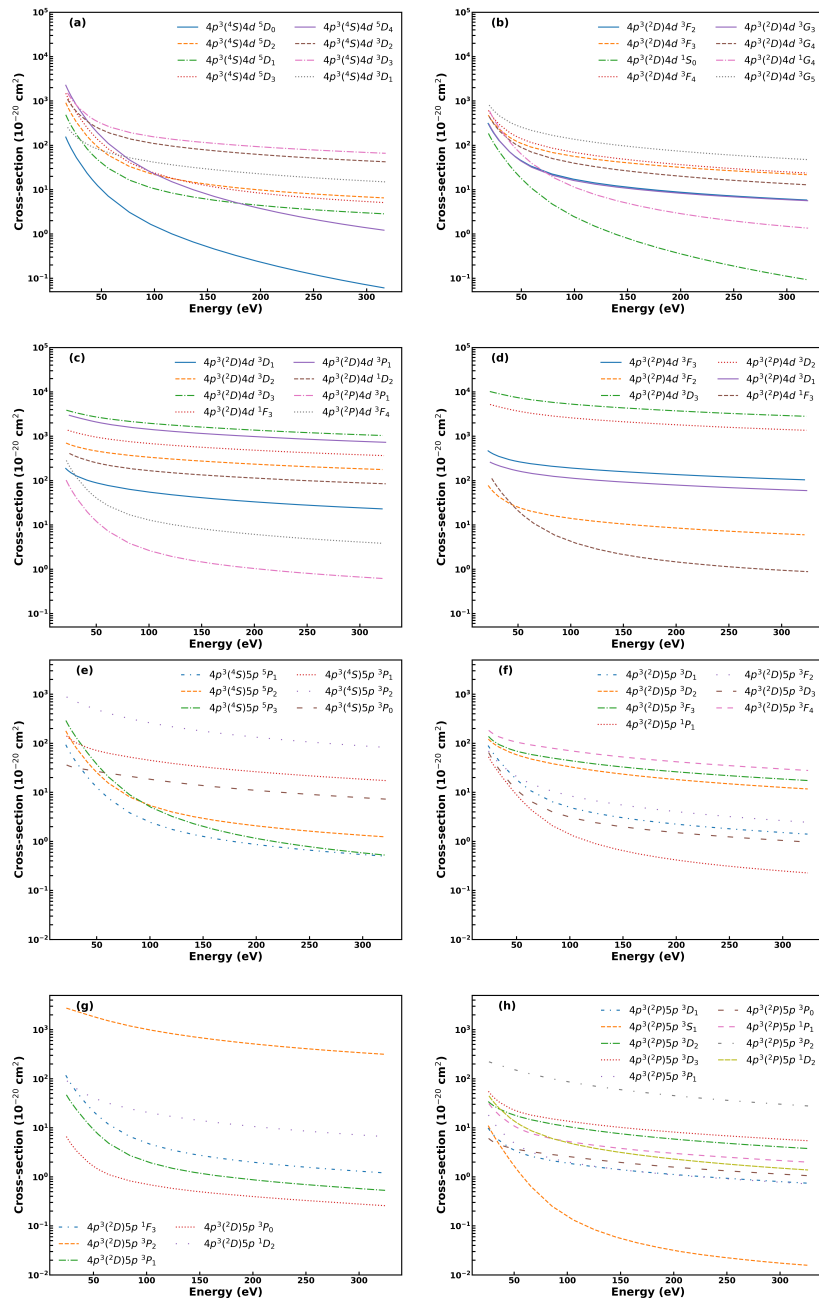


Figure 3. EIE cross-sections for transitions from the $4s^2 4p^4 \ ^3P_2$ level of Kr III to higher excited levels belonging to (a–d) $4s^2 4p^3 4d$ and (e–h) $4s^2 4p^3 5p$ configurations.

3.3. CR Model for Kr III

For building the present model, we took into account population transfer among the various levels by considering (i) radiative decay among the fine structure levels generated from $4s4p^5$, $4s^24p^34d$, $4s^24p^35d$, $4s^24p^35s$, $4s^24p^35p$, $4s^24p^36s$, $4s^24p^36p$, $4s^24p^37s$, and $4s^24p^37p$ configurations; (ii) electron impact excitation from ground and first four excited states to all the above-mentioned levels; and (iii) electron impact ionization from the ground state of Kr III to Kr IV calculated using the Flexible Atomic Code (FAC) [30]. In addition, reverse processes, such as photo-excitation, de-excitation, and three-body recombination, were also considered. Overall, the atomic structures of 192 levels were considered when developing the present CR model. In most CR models, the contribution of the ground level was sufficient to provide a feasible prediction of plasma parameters. However, to provide a detailed model that can be more effective for low-temperature plasma diagnosis, we considered extended contributions by including metastable states corresponding to the $4s^24p^4$ configuration. Next, considering a quasi-static approximation, for a level j , we defined the particle balance equation as,

$$0 = - \left[F_{j+}(T_e)n_e + \sum_{j>i} A_{ji} + \sum_{i=1, i \neq j}^N C_{ji}(T_e)n_e \right] n_j + \left[\sum_{i=1, i \neq j}^N C_{ij}(T_e)n_e + \sum_{i>j} A_{ij} \right] n_i + F_{+j}(T_e)n_en_+n_e. \quad (4)$$

Here, n_e and $n_{(j/i)}$ are the electron density and population of level j/i , respectively. n_+ is the density of Kr IV. A_{ij} and A_{ji} are the radiative transition rates of transition from i to j and j to i , respectively. C_{ij}/F_{j+} are the collisional excitation/ionization coefficients. C_{ji}/F_{+j} are the de-excitation/three body recombination coefficients. The above equation perfectly combines the collisional excitation/de-excitation, ionization/recombination, and radiative processes responsible for determining the population in optically thin low-temperature plasma. The rate coefficients for the reverse processes are calculated using the principle of detail balance [5]. For all of the considered levels, Equation (4) is solved as a function of electron densities (n_e) and temperatures (T_e). Following this, the emission intensity, I_{ji} , is calculated as:

$$I_{ji} = n_j A_{ji} \frac{hc}{\lambda_{ji}}, \quad (5)$$

for a wide range of T_e and n_e . Further, to validate the present model, we coupled our simulated intensities with the experimental intensities of Belmonte et al. [8]. They reported transition rates of 62 lines emitted by a low-pressure pulsed discharged plasma of Kr III. They selected 12 lines (mentioned in Table 1 of [8]) as reference lines for which they used the technique of the Boltzmann plot and obtained the plasma temperature at different instances of plasma lifetime. However, upon requesting data from the authors, the intensities of only eight lines were available, which are mentioned in Table 2.

For analysis, we calculated the normalised intensities from both the present model and the measurements [8] as,

$$I_{\lambda_i, \text{expt}}^{\text{NR}}(\text{model}) = \frac{I_{\lambda_i, \text{expt}}(\text{model})}{\sum_{\lambda_i=1,8} I_{\lambda_i, \text{expt}}(\text{model})} \times 100. \quad (6)$$

It is worth mentioning that the normalised intensities for the experimental observations of [8] were calculated using intensities recorded at plasma lifetime instance of 100 μs . The agreement between the present and experimental intensities was measured based on the least-square deviation principle. We define the deviation parameter, Δ ,

$$\Delta = \sum_{i=1}^8 \left(I_{\lambda_i, \text{expt}}^{\text{NR}} - I_{\lambda_i, \text{model}}^{\text{NR}} \right)^2. \quad (7)$$

Table 2. Wavelength (in the vacuum) of lines observed in the experiment of [8] along with the associated level labels and their energies.

Line Index	Wavelength (nm)		Level		Energies (eV) (NIST)	
	NIST	Present	Upper	Lower	Upper Level	Lower Level
L1	309.716	328.984	$4s^2 4p^3(^4S)5p^3P_2$	$4s^2 4p^3(^4S)4d^3D_2$	22.32744	18.325429
L2	312.246	333.544	$4s^2 4p^3(^2P)5p^1P_1$	$4s^2 4p^3(^2P)5s^3P_2$	26.31735	22.347791
L3	315.175	324.804	$4s^2 4p^3(^2P)5p^3D_2$	$4s^2 4p^3(^2P)4d^3P_2$	25.851944	21.919259
L4	322.062	337.629	$4s^2 4p^3(^2P)5p^3P_1$	$4s^2 4p^3(^2P)5s^3P_0$	25.94796	22.09938
L5	322.224	339.683	$4s^2 4p^3(^2P)5p^3P_1$	$4s^2 4p^3(^2P)5s^3P_1$	25.94796	22.1013
L6	327.165	344.554	$4s^2 4p^3(^4S)5p^3P_1$	$4s^2 4p^3(^4S)4d^3D_1$	22.271137	18.482554
L7	344.871	373.300	$4s^2 4p^3(^2P)5p^3D_1$	$4s^2 4p^3(^2P)5s^3P_1$	25.695354	22.1013
L8	351.455	362.983	$4s^2 4p^3(^2D)5p^1D_2$	$4s^2 4p^3(^2D)4d^3D_3$	25.15589	21.629161

In our study, the electron temperature and electron density were systematically varied to determine each combination's deviation parameter. The optimal plasma parameters were identified by selecting the combination of (n_e, T_e) that minimized the deviation parameter. To achieve this, first, we tried to find the best range of density where we observed the least deviation parameters. We considered a wide density grid from 10^{16} m^{-3} to 10^{24} m^{-3} and observed the least deviation around 10^{22} m^{-3} . Then, we used a finer grid of density variation in the range from $(1-18) \times 10^{22} \text{ m}^{-3}$, and varied the temperature with a very fine grid in this density range. The deviation in the present and experimental intensities over a wide temperature grid and above densities is shown in Figure 4. No significant variation in the Δ value was observed within this density range. However, we noted a very sensitive variation in the deviation parameter with temperature, with values ranging from a maximum of 4000 to as low as 35.

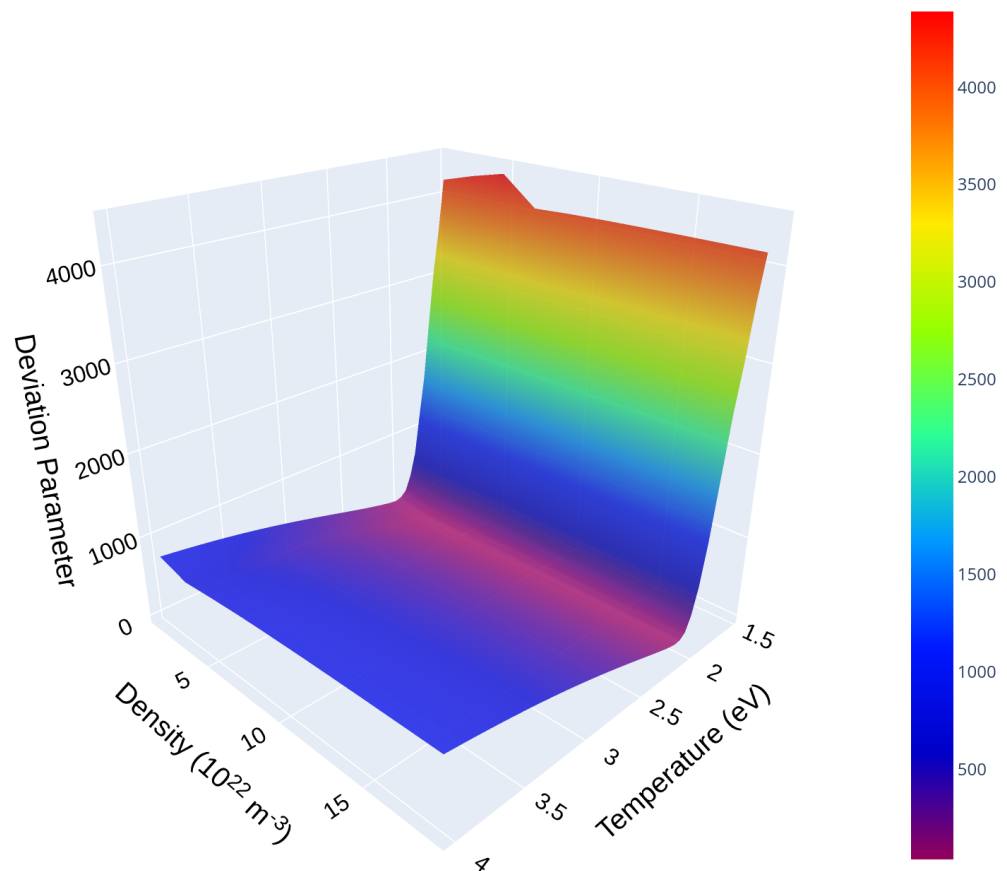


Figure 4. The variation in deviation parameter for a range of temperatures and densities.

Using the Boltzmann plot analysis, Belmonte et al. [8] mentioned that the plasma temperature at the instance of 100 μ s lifetime is 2.26 ± 0.23 eV and the range of their plasma density is $(1.7\text{--}3.2) \times 10^{22} \text{ m}^{-3}$. Examining Figure 4, the model predicted temperature for this plasma of Kr III was 2.05 eV at an electron density of $2.96 \times 10^{22} \text{ m}^{-3}$, which nearly agreed with the experimental value. Moreover, in Figure 5, we present the comparison of the model and experimental normalised intensities for the considered lines (see Table 2). Our simulated intensities nearly followed the same pattern as of [8], with the L1 line showing the maximum intensity and the least for L5. The deviation parameter values for the lines were as follows: L1 (0.3), L2 (12.2), L3 (0), L4 (20.9), L5 (0.2), L6 (0.5), L7 (0.2), and L8 (0). Clearly, the simulated intensities for the L2 and L4 lines do not agree well. The model intensity for L2 was over-predicted, whereas for L4, the model intensity was below the experimental values. Irrespective of this, our model was able to make a good prediction of T_e and n_e .

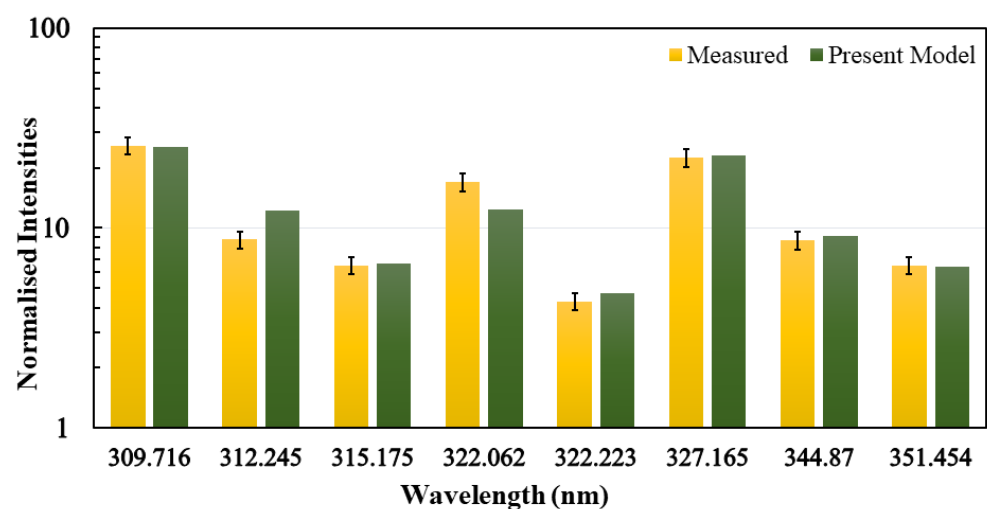


Figure 5. Comparison of normalized measured intensities of [8] with the intensities stimulated from the present CR model.

4. Conclusions

A detailed collisional radiative model was built for application in diagnosing a low-temperature plasma of Kr III. Calculations of the energies and transition parameters were carried out using the MCDHF approach to develop the model. The obtained results were compared with the NIST and previously reported values. Further, using these bound state functions and employing RDW approximation, EIE cross sections for the transition from the lowest five levels were calculated for an incident electron energy range from threshold to 300 eV. To depict the application and reliability of the model and the calculated parameters, our simulated intensities were coupled with the measured intensities of eight lines [8]. Using this and employing the principle of least deviation, we predicted the plasma temperature as 2.05 eV compared to the experimental value of 2.26 ± 0.23 eV at 100 μ s instance of the plasma lifetime. The density predicted by our model was $2.96 \times 10^{22} \text{ m}^{-3}$, which was in the experimental range of $(1.7\text{--}3.2) \times 10^{22} \text{ m}^{-3}$. This agreement assures that the parameters and the model created in the study can be used for plasma diagnosis.

Author Contributions: S.R.: formal analysis, conceptualization, investigation, methodology, writing—original draft. L.S.: resources, funding acquisition, supervision, writing—review and editing. All of the authors have read and agreed to the published version of the manuscript.

Funding: This research is funded by IAEA through Research Contract No.: 26504.

Data Availability Statement: Data will be made available upon reasonable request.

Acknowledgments: S R gratefully acknowledges the Ministry of Education for the Research Fellowship. L S thanks IAEA, Vienna, for sanctioning the IAEA Research Contract No. 26504. We both are grateful to M T Belmonte for sharing the experimental data in electronic form.

Conflicts of Interest: The authors declare no conflict of interest.

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