Journal of Atomic, Molecular, Condensate & Nano Physics Vol. 3, No. 2, pp. 137–150, 2016 ISSN 2349-2716 (online); 2349-6088 (print) Published by RGN Publications



Multiconfigurational Dirac-Fock Energy Levels and Radiative Rates for Kr XX

Research Article

Narendra Singh

Department of Physics, Shyamlal College (University of Delhi), Shahdara, Delhi 110032, India nsingh76@yahoo.co.in

Abstract. In present calculations, energy levels and radiative properties are reported for transitions in Cl-like Kr. For these calculations, the fully relativistic multiconfigurational Dirac-Fock (MCDF) approach is employed by including 54 configurations (generating 5370 levels) and the Breit and quantum electrodynamics effects. To assess the accuracy of presented results, calculations have also been performed for energy levels using the fully relativistic flexible atomic code (FAC) and comparisons are made with the existing experimental and theoretical data. Energies are reported for the lowest 100 levels corresponding to the configurations $3s^23p^5$, $3s^3p6$, $3s^23p^43d$, $3s3p^53d$, $3s^23p^33d^2$ and radiative rates are provided for E1 and M2 transitions from ground state.

Keywords. Atomic data; Cl-like Kr; Multiconfigurational Dirac-Fock method

PACS. 32.70.Cs; 32.10.Fn

Received: January 13, 2016 Accepted: August 20, 2016

Copyright © 2016 Narendra Singh. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

1. Introduction

Krypton has attracted a great deal of interest in various studies as emission lines arising from krypton ions are increasingly being observed in high temperature plasma [1]. It is also being used in tokamak fusion plasma [2,3] as an injected impurity. Therefore, the study of krypton ions has become more important in view of forthcoming ITER Project. In order to estimate the power loss and to analyse observations, atomic data, such as energy levels, transition probabilities, line strengths, oscillator strengths etc. are required. With this view, data for Cl-like krypton (Kr XX) have been provided.

In past years, a remarkable work has been provided for Cl-like ions. CIV3 code has been used by Hibbert, Mohan and others for Co XI [4], Ar II-Ge XVI [5], K III-Sc V [6], Cu XIII [7] and Fe X [8] while Bhatia and Doschek [9] has used Superstructure code. Huang et al. [10] also preformed energy level and transition probability calculations using MCDF approach. Cowan's code has been used for Ar II-Fe X by Fawcett [11]. R-matrix method has been used by Berrington et al. [12] for Cl-like ions. Experimental measurements have also been performed for Cl-like ions Ti VI [13], Ar II [14] and for Ni XII, Fe X and Cu XII [15] using different light sources. Kaufman et al. [16] generated spectra of Cl-like Cu to Mo in tokamak and laser produced plasmas. Various theoretical and experimental works and their compilation have been provided for Cl-like Kr ion [17–22]. Rodrigues et al. [17] calculated atomic binding energies of Cl-isoelectronic sequence including Cl-like Kr. Ionization potential of Kr XX was calculated by different authors [23–25] using different approaches. Samii and Macdonald [26] calculated transition wavelengths, energies and oscillator strengths for electric dipole transitions in Cllike Kr. Huang et al. [10] performed calculations for energy levels and transition probabilities for energy levels and transition probabilities for several ions including Kr XX. Baluja and Aggarwal [19] calculated lifetime for 3s²3p^{5 2}P_{3/2}-²P_{1/2} transition. Wyart and TFR group [27] identified four lines of 3s²3p⁵-3s²3p⁴3d array. Denne *et al.* [28] and Roberts *et al.* [29] observed spectral lines from magnetic dipole transitions in $3s^23p^x$ configurations in Princeton large tokamak discharge and in texas experimental tokamak respectively.

The need of highly accurate atomic data arises from the fact that the accurate measurement of data is difficult at extreme conditions due to limited number of experimental techniques. Therefore one has to depend on theoretical data. Thus, a large amount of data for Cl-like Kr has been furnished which belongs to $3s^23p^5$, $3s3p^6$, $3s^23p^43d$, $3s3p^53d$, $3s^23p^33d^2$ configurations. The radiative data for E1 and M2 transition from the ground state to all exited states has also been provided. For present calculations, the multi-configuration Dirac-Fock (MCDF) method, which was developed by Grant et al. [30] is adopted. This package was later revised by many authors under names GRASP1 [31], GRASP2 [32] and Grasp2k [33]. The version GRASP0 [34] used in this calculation include all the correlation effects as well as Breit and QED corrections. It has been successfully used by us and others [35–39, 41] to calculate atomic data for different ions (including Cl-like ions). The result has been compared with other available results obtained from experimental measurement and theoretical calculations [35–41]. Calculated results with MCDF method are in good agreement with FAC calculation as well as with other available results, which shows the reliability of presented results. The present computations may be useful for understanding fusion plasma and in modelling of plasma.

2. Theoretical Method

To perform these calculations, General purpose relativistic atomic structure package (GRASP) a fully relativistic MCDF method revised by Norrington [34] formerly made by Grant *et al.* [30]. QED corrections due to self energy and vacuum polarization effects have adopted

and Breit corrections have also been considered because of swapping of virtual photons as a first order perturbation theory. As the elaborate description and explication of this technique has been presented elsewhere, therefore only brief key points of this method are discussed here. The methodology of extended average level (EAL) to acquire radial wave functions in which weighted trace of the Hamiltonian matrix is minimized at the time of self consistent field (SCF) computations have employed. For a system of N electron atom or ion, Dirac-Coulomb Hamiltonian in MCDF method is given as follows

$$\hat{H}^{DC} = \sum_{i=1}^{N} \hat{H}_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{|\hat{r}_i - \hat{r}_j|}$$
(2.1)

where \hat{H}_i , the one electron Hamiltonian is given by

$$\widehat{H}_i = c \vec{\alpha}_i \cdot \vec{p}_i + \beta m c^2 + V_{nuc} \tag{2.2}$$

The first two terms in the above equation signify kinetic energy of an electron and the last term depicts the Coulomb potential of the nucleus. α and β are 4×4 Dirac matrices and c is the speed of light.

The N-electron wave functions, the sum of products of central-field Dirac orbitals can be written in matrix form as follows

$$\varphi_{nkm} = \frac{1}{r} \begin{bmatrix} P_{nk}(r) & \chi_{km}(\theta, \varphi, \sigma) \\ -iQ_{nk}(r) & \chi_{-km}(\theta, \varphi, \sigma)) \end{bmatrix}$$
(2.3)

where $Q_{nk}(r)$ and $P_{nk}(r)$ are large and small components of one electron radial wave-functions. $k = \pm (j + \frac{1}{2})$ for $l = j \pm \frac{1}{2}$.

k and m are the relativistic angular quantum number and m is also the projection of total angular momentum j.

The spinor spherical harmonic function is given by

$$\chi_{km}(\theta,\varphi) = \sum_{\sigma=\pm\frac{1}{2}} \left\langle lm - \sigma \frac{1}{2}\sigma \mid l\frac{1}{2}jm \right\rangle Y_l^{m-\sigma}(\theta,\varphi)\varphi^{\sigma}$$
(2.4)

 χ_{km} has 2 components. In above equation, $Y_l^{m-\sigma}(\theta, \varphi)$ is spherical harmonic function of degree l and order $m - \sigma$. θ is polar angle ranges from 0 to π and φ is azimuthal angle ranges from 0 to 2π and σ is the electron spin *z*-projection quantum number.

An atomic state function (ASF) ψ for N electron system is built by the linear combination of n_c electronic configuration state functions (CSFs)

$$|\psi_{\mu}(PJM)\rangle = \sum_{i=1}^{n_{c}} C_{i}(\mu) |\gamma_{i}(PJM)\rangle$$
(2.5)

where $\gamma_i(PJM)$ are CSFs which signify a particular state with a given angular momentum (J, M) and parity P and $C_i(\mu)$ are the expansion mixing co-efficients for each CSF and satisfy the relation

$$(C_i(\mu))^+ C_j(\mu) = \delta_{ij}$$
(2.6)

Journal of Atomic, Molecular, Condensate & Nano Physics, Vol. 3, No. 2, pp. 137–150, 2016

Such that ASFs satisfy the condition of orthonormality. μ represents the orbital occupation numbers, coupling, etc.

The expectation value of Dirac-Hamiltonian is energy of the N electron atom or ion and it is defined as

$$E_{\alpha}^{PJM} = \langle \psi_{\mu}(PJM) | H^{DC} | \psi_{\mu}(PJM) \rangle$$

$$= \sum_{ij} C_{i}^{*}(\mu) C_{i}(\mu) \rangle \gamma_{i}(PJM) | H^{DC} | \gamma_{j}(PJM) \rangle$$

$$= (C_{\mu}^{DC})^{\dagger} H^{DC} C_{\mu}^{DC}$$
(2.7)

The elements of Dirac Hamiltonian H^{DC} are given by

$$H_{rs}^{DC} = \langle \gamma_r(PJM) | H^{DC} | \gamma_s(PJM) \rangle$$
(2.8)

By applying the condition of normalization

$$(H^{DC} - E^{DC}_{\mu}I)C^{DC}_{\mu} = 0 (2.9)$$

where in equation (2.9), I is the identity matrix and E_{μ}^{PJM} are the eigenvalues of H^{DC} .

3. Results and Discussion

3.1 Energy Levels

For highly charged ions, the basic procedure for the determination of accurate and reliable atomic data is configuration interaction. Therefore, in this work, the energy values of $(1s^2 2s^2 2p^6) 3s^2 3p^5$, $3s 3p^6$, $3s^2 3p^4 3d$, $3s 3p^5 3d$ and $3s^2 3p^3 3d^2$ configuration using $(1s^2 2s^2 2p^6) 3s^2 3p^5$, $3s 3p^6$, $3s^2 3p^4 3d$, $3s^2 3p^3 3d^2$, $3p^6 3d$, $3s 3p^2 3d^4$, $3s^2 3p^4 4d$, $3s^2 3p^3 3d4p$, $3s^2 3p^3 3d4f$, $3s 3p^5 4p$, $3s 3p^5 4f$, $3s^2 3d^5$, $3p^2 3d^5$, $3s^2 3p^4 3d^2$, $3s 3p^5 3d$, $3s 3p^3 3d^3$, $3s^2 3p 3d^4$, $3p^5 3d^2$, $3s^2 3p^4 4p$, $3s^2 3p^4 4f$, $3s^2 3p^3 3d4s$, $3s^2 3p^3 3d4d$, $3s 3p^5 4d$, $3s 3p^5 3d^3$, $3s^2 3p 3d^4$, $3p^5 3d^2$, $3s^2 3p^4 4p$, $3s^2 3p^4 4f$, $3s^2 3p^3 3d4s$, $3s^2 3p^3 3d4d$, $3s 3p^5 5d$, $3s 3p^5 5d$, $3s^2 3p^4 5d$, $3s^2 3p^4 5d$, $3s^2 3p^4 5g$, $3p^6 4s$, $3p^6 4d$, $3s 3p^5 5s$, $3s 3p^5 5f$, $3s 3p^5 5f$, $3s 3d^6$, $3d^7$, $3s^2 3p^4 5d$, $3s^2 3p^4 5d$, $3s^2 3p^4 6d$, $3s^2 3p^4 6f$, $3s^2 3p^4 6g$, $3s^2 3p^4 4s^2$, $3s 3p^4 4s^2$, $3s 3p^4 4s^2$, $3s 3p^4 4s^2$, $3s 3p^4 4s^2$, $3s^2 3p^4 6d$, $3s^2 3p^4 6d$, $3s^2 3p^4 6f$, $3s^2 3p^4 6g$, $3s^2 3p^4 6g$, $3s^2 3p^4 6g$, $3s^2 3p^4 6d$, $3s^2 3p^4 6f$, $3s^2 3p^4 6g$, $3s 3p^4 3d4s$ configurations have been provided. The Ne-like $[1s^2 2s^2 2p^6]$ core treated as an inactive core.

In Table 1, the fine-structure energies calculated by MCDF method along with the compositions of the wave functions in LSJ coupling for Cl like Kr are reported. Lifetimes of all excited levels have also been presented. In the LSJ notation, configurations state functional (CSF) for $3s^23p^43d$ configuration is given only by LS term and seniority of $3p^4$ subshell and the final LS term. In "composition" column of Table 1, firstly the percentage of basis state corresponding to level's name; next the second largest percentage together with the related basis state are given.

In present MCDF calculations, mixing among some levels in LSJ coupling is very strong. For example for Cl-like Kr, $3s^2 3p^4 (2^3P) 3d 2^F$ is strongly coupled with $3s^2 3p^4 (2^3P)3d 4^F$ and $3s^2 3p^4$ (1₂D) $3d2^G$ with their percentage compositions as 34.9%, 33.2% and 25.4% respectively. Similarly *I* found that 27.1% of $3s^2 3p^4$ ($2^3 P$) $3d 4^F$ level strongly couples with 22.4% of level $3s^2 3p^4 (3_2 P) 3d 4^P$ level. Similarly there are many other cases, as can be seen from Table 1. Therefore, the explicit identification of the levels is very difficult.

In Table 2, energies in Rydberg for 100 levels belonging to the configurations $(1s^22s^22p^6)$ $3s^23p^5$, $3s3p^6$, $3s^23p^43d$, $3s3p^53d$ and $3s^23p^33d^2$ for Cl-like Kr have been reported. The contribution to excitation energy from QED and Breit effect are also reported in this table. It can be seen from Table 2 that the *DC* contribution is the largest, with Breit interaction providing a significant correction. The effect of QED correction is negligible as compared as Breit corrections. In Table 2, comparisons have also been made between calculated result with the data compiled by National Institute of Standards and Technology (NIST) [42]. For the level $3s^23p^5$ (${}^{2}P_{1/2}$), the disagreement between calculated MCDF energies and NIST energies is about 0.1%. MCDF results agree within 1.4% with NIST for all 3s⁴ 3p⁴ 3d levels. This is due to presence of strong mixing in present calculation. Overall, a good agreement between MCDF results and NIST results have achieved. To scrutinize the reliability of calculated results, calculations for energy values have also performed using fully relativistic distributed wave method FAC (flexible atomic code). This method allows the user to determine atomic parameters in a short time limit due to its higher efficiency. From Table 2, one can see that the result from both calculations (MCDF and FAC) are in good agreement with each other and hence confirms the reliability of presented results.

A point worth mentioning here is that results for many new spectral lines, which are not listed in the NIST tables have presented. It can be seen that results for $3s^2p^6$, $3s^3p^53d$ and $3s^23p^3d^2$ for Kr XX has been listed which are not presented by any author. Also, many new levels for $3s^23p^43d$ which have not been reported so far has also being reported.

3.2 Radiative Rates

In Table 3 and 4, the transitions wavelength (λ in Å), radiative rate (A_{ji} in s^{-1}), oscillator strength (f_{ij} , dimensionless) and line strengths (s in a.u.) for E1 and M2 transitions from the $3s^23p^5 \ ^2P_{3/2}$ levels have been presented. The results are presented in only in length form as the results in babushkin gauge is assumed to be more accurate than in coulomb gauge. The indices for the notation of lower level i and upper level j are mentioned in the first column of Table 1. Further in these tables, comparisons have made between my calculated transition wavelengths and radiative rates using MCDF method with NIST and Huang *et al.* [10]. This comparison will give credence to the accuracy and reliability of calculated results. One can see from Table 3 that my reported results matches well with NIST and Huang [10] results. Also for most of the transitions the order radiative rates are same as Huang [10], which confirm the reliability of my work. Further, some of the levels identified by us differ from Huang *et al.* [10]. I believe that this is due to strong mixing present.

	Label	J	Level (Ryd)	Lifetimes	Composition
1	$3s^23p^{5\ 2}P^{0}$	3/2	0	-	97.4
2	$3s^23p^{5\ 2}P^{0}$	1/2	0.79397	8.43E-05	97.2
3	$3s3p^{6}$ ² S	1/2	5.16521	7.88E-11	70.9+26.4(26)
4	$3s^23p^4({}_2 {}^3P)3d {}^4D$	5/2	6.37505	2.52E-08	77.8
5	$3s^23p^4({}_2 {}^3P)3d {}^4D$	3/2	6.39547	1.01E-08	69.4
6	$3s^23p^4(2^3P)3d^4D$	7/2	6.44711	2.58E-03	80.6
7	$3s^2 3p^4 ({}_2{}^3P) 3d {}^4D$	1/2	6.4968	3.38E-09	59.9+16.9(11)
8	$3s^23p^4(2^3P)3d^4F$	9/2	6.81047	5.37E-03	81.2+17.1(21)
9	$3s^23p^4(2^{3}P)3d^{2}F$	7/2	6.90363	4.66E-03	34.9+33.2(17)+25.4(20)
10	$3s^23p^4({}_2^{3}P)3d {}^4P$	3/2	7.04919	8.75E-10	24.4(25)+21.9+19.2(14)
11	$3s^23p^4(2^1D)3d^2P$	1/2	7.04842	3.22E-09	34.2(7)+32.9+30(30)
12	$3s^23p^4(2^{3}P)3d^{4}P$	1/2	7.166	1.33E-10	85.7
13	$3s^23p^4(2^{3}P)3d^{4}F$	5/2	7.24728	5.28E-10	81.2
14	$3s^23p^4(2^{3}P)3d^{4}F$	3/2	7.29103	7.74E-10	27.1+22.4(10)+17.9(18)
15	$3s^23p^4({}_2^{-1}D)3d^{-2}D$	3/2	7.32474	3.32E-10	33.1(14)+25.2
16	$3s^23p^4(2^3P)3d^4P$	5/2	7.41733	8.42E-10	51.3+16.8(22)
17	$3s^23p^4(2^{3}P)3d^{4}F$	7/2	7.47268	1.32E-04	48.2+20.3(9)
18	$3s^23p^4(2^1D)3d^2P$	3/2	7.60879	4.22E-09	37.7(10)+21.4+20.1(28)
19	$3s^23p^4(2^1D)3d^2D$	5/2	7.68483	8.24E-10	39.6+18.8(16)+17.3(29)
20	$3s^23p^4(2^1D)3d^2G$	7/2	7.70725	1.50E-04	57.6+24.4(9)
21	$3s^23p^4({}_2^{-1}D)3d^{-2}G$	9/2	7.79717	1.34E-04	81+17(8)
22	$3s^23p^4(2^{3}P)3d^{2}F$	5/2	7.82313	1.08E-09	53.7+28(23)
23	$3s^23p^4({}_2^{-1}D)3d^{-2}F$	5/2	8.12398	5.19E-10	54.9+21.7(19)
24	$3s^23p^4(2^1D)3d^2F$	$\frac{3}{2}$	8.32666	7.45E-05	72.6+18.1(9)
25	$3s^23p^4(_0 {}^1S)3d {}^2D$	3/2	8.65136	3.66E-11	48.2+21(15)
26	$3s^23p^4(2 {}^1D)3d {}^2S$	1/2	8.96243	2.83E-12	64.8+22.9(3)
27	$3s^23p^4(_0 {}^1S)3d {}^2D$	5/2	9.05481	4.47E-11	67.7
28	$3s^23p^4(2^3P)3d^2P$	3/2	9.27627	3.46E-12	44+28.4(18)
29	$3s^23p^4(2^3P)3d^2D$	5/2	9.3226	3.06E-12	65.8+25.1(19)
30	$3s^23p^4(2^3P)3d^2P$	1/2	9.56859	3.58E-12	48.7+42.8(11)
31	$3s^23p^4({}_2{}^3P)3d {}^2D$	3/2	10.0193	3.03E-12	53.1+18.1(25)
32	$3s3p^{5}(^{3}P)3d^{4}P$	1/2	11.2522	1.09E-10	81.2
33	$3s3p^{5}(^{3}P)3d^{4}P$	3/2	11.3598	1.09E-10	77.1
34	$3s3p^{5}(^{3}P)3d^{4}P$	$\frac{5/2}{5/2}$	11.5681	1.06E-10	70.2
35	$3s3p^{5}(^{3}P)3d^{4}F$	$\frac{3}{2}$ 9/2	11.8388	6.10E-11	85.2
36	$3s3p^{5}(^{3}P)3d^{4}F$	$\frac{3}{2}$ 7/2	11.8662	6.18E-11	69.6
30 37	$3s3p^{5}(^{3}P)3d^{4}F$	5/2	11.985	5.76E-11	63.2
38	$3s3p^{5}(^{3}P)3d^{4}F$	$\frac{3}{2}$ $\frac{3}{2}$	12.1287	5.37E-11	60.1
30 39	3s3p ⁵ (³ P)3d ⁴ D	$\frac{3/2}{1/2}$	12.3352	6.73E-11	54.5
40	$3s3p^{5}(^{3}P)3d^{4}D$	$\frac{1/2}{7/2}$	12.3552 12.351	9.11E-11	39.7+38.7(42)
40 41	3s3p ⁵ (³ P)3d ² D	5/2	12.331 12.4679	9.11E-11 6.96E-11	39.7+38.7(42) 30.4+26.4(44)
41 42	$3s3p^{5}(^{3}P)3d^{2}F$	$\frac{5}{2}$ 7/2	12.4079	7.50E-11	30.4+20.4(44) 27.4(40)+26.4
42 43	$3s3p^{5}(^{3}P)3d^{4}D$	3/2		6.72E-11	45.8
	$3s3p^{5}(^{3}P)3d^{2}F$	$\frac{3}{2}$ 5/2	12.5161 12.5992		
44 45	$3s3p^{5}(^{3}P)3d^{2}D$			1.12E-10	24.5(51)+23.7(41)+21.7
45 46	3s3p ⁵ (³ P)3d ² P 3s3p ⁵ (¹ P)3d ² P	3/2	12.6602	6.36E-11	48.7
46	$3s^{2}3p^{3}({}_{3}{}^{4}S)3d^{2}({}_{2}{}^{3}F)^{6}F$	$\frac{1}{2}$	12.7872	3.19E-11	27.5+25.7(84)
47	$3s^{2}3p^{3}(_{3} {}^{4}S)3d^{2}(_{2} {}^{3}F)^{6}F$ $3s^{2}3p^{3}(_{3} {}^{4}S)3d^{2}(_{2} {}^{3}F)^{6}F$	5/2	12.9857	2.05E-10	70.2
48 49	$3s^{2}3p^{3}(_{3} + S)3d^{2}(_{2} + F)^{6}F$ $3s^{2}3p^{3}(_{3} + S)3d^{2}(_{2} + F)^{6}F$	3/2 1/2	12.9917	2.11E-10	75.5
	39 30 (a + S)30 4 (a 9 K) 9 K	1/2	13.0077	1.73E-10	82.6

Table 1. MCDF	r energies (in Ryd.)), lifetimes (in s), and	d mixing coefficients	s of levels in Cl-like Kr.

(Table Contd.)

~ 1	2 ³ 5/ ³ D) 2 1 ² D	- 10	10.0105		
51 50	$3s^3p^5({}^3P)3d {}^2F$	5/2	13.0197	7.92E-11	32.5
52	$3s^{2}3p^{3}(_{3}4S)3d^{2}(_{2}3F)^{6}F$	9/2	13.0652	7.62E-10	85.4
53	$3s^2 3p^3 (_3 {}^4S) 3d^2 (_2 {}^3F) {}^6F$	11/2	13.1206	5.81E-09	85.9
54	$3s^3p^5(^1P)3d^2P$	3/2	13.2458	4.04E-11	21.3+16.6(45)
55	$3s^3p^5(^1P)3d^2F$	5/2	13.3406	4.70E-11	39.3
56	$3s^{2}3p^{3}(_{3}{}^{4}S)3d^{2}(_{2}{}^{3}P){}^{6}P$	3/2	13.3726	2.49E-10	77.6
57	$3s^23p^3(_3 {}^4S)3d^2(_2 {}^3P) {}^6P$	7/2	13.3899	2.17E-10	61.5
58	3s ² 3p ³ (₃ ⁴ S)3d ² (₂ ³ P) ⁶ P	5/2	13.416	2.80E-10	80.3
59	$3s^23p^3(_3{}^2D)3d^2(_2{}^3P){}^4F$	3/2	13.5266	1.38E-10	15.3
60	3s3p ⁵ (¹ P)3d ² F	7/2	13.5537	4.61E-11	33.8
61	3s ² 3p ³ (3 ² D)3d ² (2 ³ P) ⁴ P	1/2	13.5969	2.45E-10	34.1
62	$3s^23p^3(_3{}^2D)3d^2(_2{}^3F)^4G$	5/2	13.6706	9.54E-11	27
63	$3s^23p^3(_3^2D)3d^2(_2^3F)^4G$	7/2	13.7162	1.38E-10	19.4
64	3s3p ⁵ (¹ P)3d ² D	3/2	13.7668	2.72E-11	40.8
65	$3s^23p^3(_3^4S)3d^2(_2^1D)^4D$	5/2	13.7971	9.20E-11	27+19(62)
66	$3s^23p^3(_3^4S)3d^2(_2^1D)^4D$	7/2	13.8185	$9.65 \text{E}{-}11$	23.8
67	$3s^23p^3(_3^4S)3d^2(_2^1D)^4D$	3/2	13.8301	1.22E-10	33.3
68	3s3p ⁵ (¹ P)3d ² D	5/2	13.8874	3.93E-11	40.6
69	$3s^23p^3(_3^4S)3d^2(_2^1D)^4D$	1/2	13.8974	5.82E-11	54.3
70	$3s^23p^3(_3^2D)3d^2(_2^3P)^4P$	5/2	13.9407	1.92E-10	14.7
71	$3s^23p^3(_3^2D)3d^2(_2^3F)^4H$	7/2	13.9372	1.38E-10	37.2
72	$3s^23p^3(_3^2D)3d^2(_2^3P)^4P$	3/2	13.9421	2.17E-10	27.2
73	$3s^23p^3(_3^2D)3d^2(_2^3F)^4G$	9/2	13.9438	3.68E-10	52.7
74	$3s^23p^3(_3^2D)3d^2(_2^3F)^4H$	9/2	14.0025	2.62E-10	45.2
75	$3s^23p^3(_3^2D)3d^2(_2^3F)^4G$	11/2	14.0305	6.04E-10	41.5
76	$3s^23p^3(_3^4S)3d^2(_2^3P)^4P$	5/2	14.0733	4.03E-10	23.7(70)+17
77	$3s^23p^3(_3^2D)3d^2(_2^3P)^4F$	7/2	14.1423	5.85E-10	39.7
78	$3s^23p^3(_3^2D)3d^2(_2^3F)^4H$	11/2	14.2146	9.28E-09	62.7
79	$3s^23p^3(_3^2D)3d^2(_2^3P)^4F$	9/2	14.2681	5.87E-10	29.9+26.8(74)
80	$3s^23p^3(_3^2D)3d^2(_2^1D)^2D$	3/2	14.3005	1.75E-11	17.3
81	$3s^23p^3(_3^2D)3d^2(_2^3F)^2H$	9/2	14.3046	2.66E-10	20.8+19.1(79)
82	$3s^23p^3(_3^2D)3d^2(_2^1D)^2F$	5/2	14.3145	3.33E-11	18.3(89)+18.1
83	$3s^23p^3(_3^2D)3d^2(_2^1D)^2F$	7/2	14.349	8.05E-11	19.8
84	3s3p ⁵ (³ P)3d ² P	1/2	14.3731	4.01E-12	45.3
85	3s3p ⁵ (³ P)3d ² P	3/2	14.4526	3.93E-12	51
86	$3s^23p^3(_3^2D)3d^2(_2^3F)^4H$	13/2	14.4536	8.17E-04	97.8
87	$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^2H$	11/2	14.4663	1.05E-09	29.9+24.4(78)
88	$3s^23p^3(_1^2P)3d^2(_2^3F)$	7/2	14.4921	2.98E-11	19.7+17.5(91)
89	$3s^{2}3p^{3}(_{1}^{2}P)3d^{2}(_{2}^{3}F)$ ⁴ G	5/2	14.5339	1.89E-11	14.7
90	$3s^{2}3p^{3}(_{3}{}^{2}D)3d^{2}(_{2}{}^{1}D){}^{2}D$	5/2	14.5683	2.80E-11	18.8
91	$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{1}D) {}^{2}G$	7/2	14.6489	2.50E-11	31.5
92	$3s^23p^3(_3^2D)3d^2(_2^1D)^2G$	9/2	14.7008	3.96E-11	42.5
93	$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^4F$	5/2	14.7313	1.21E-11	19.1
94	$3s^23p^3(_1{}^2P)3d^2(_2{}^3F){}^4D$	1/2	14.7783	8.68E-12	31.4
95	$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}F)$	3/2	14.7731	9.73E-12	35.8
96	$3s^23p^3(3^4S)3d^2(2^1G)^4G$	7/2	14.7723	1.45E-11	22+18.8(88)
97	$3s^{2}3p^{3}(3 2)3d^{2}(2 3) 4P$	3/2	14.8023	2.06E-11	26.8
98	$3s^23p^3(3^2D)3d^2(2^3F)^4F$	$\frac{3}{2}$ 9/2	14.8295	2.09E-11	28.5(92)+24.6
99	$3s^{2}3p^{3}(3 D)3d^{2}(2 T)^{-1}$	$\frac{11}{2}$	14.891	2.14E-11	57.9
100	$3s^{2}3p^{3}(_{3} {}^{4}S)3d^{2}(_{0} {}^{1}S) {}^{4}S$	3/2	14.8837	9.43E-11	14.2
200	55 5P (5 5)54 (0 5) 5	<i>, 1</i>	1	0.101 11	

Label	J		FAC	NIST			
		DC	DC Breit QED T				
3s ² 3p ⁵ ² P ⁰	3/2	-	-	-	-	0	0
$3s^2 3p^5 {}^2 P^0$	1/2	0.80832	-0.0155	0.00111	0.79397	0.7947	0.795
$3s3p^{6}$ ² S	1/2	5.18115	-0.0053	-0.0106	5.16521	5.1658	
$3s^23p^4(2^3P)3d^4D$	5/2	6.39499	-0.0193	-0.0006	6.37505	6.3454	
$3s^23p^4({}_2{}^3P)3d {}^4D$	3/2	6.41042	-0.0143	-0.0006	6.39547	6.3654	
$3s^23p^4({}_2{}^3P)3d {}^4D$	7/2	6.47353	-0.0259	-0.0006	6.44711	6.4179	
$3s^23p^4({}_2{}^3P)3d {}^4D$	1'/2	6.5144	-0.017	-0.0006	6.4968	6.4657	
$3s^23p^4({}_2{}^3P)3d {}^4F$	9'/2	6.83727	-0.0261	-0.0007	6.81047	6.7817	
$3s^23p^4(2^3P)3d^2F$	7'/2	6.92316	-0.0189	-0.0007	6.90363	6.8728	
$3s^23p^4(2^3P)3d^4P$	3'/2	7.06713	-0.0173	-0.0006	7.04919	7.0158	
$3s^23p^4(2^1D)3d^2P$	1/2	7.07427	-0.0259	1.1E-05	7.04842	7.0197	
$3s^23p^4(2^{3}P)3d^{4}P$	1/2	7.18614	-0.0194	-0.0007	7.166	7.1342	
$3s^23p^4(2^{3}P)3d^{4}F$	5/2	7.27361	-0.0263	-7E-05	7.24728	7.2189	
$3s^23p^4({}_2{}^3P)3d {}^4F$	3/2	7.31768	-0.0268	0.00015	7.29103	7.2598	
$3s^23p^4(2, {}^1D)3d {}^2D$	3/2 $3/2$	7.35087	-0.026	-0.00015	7.32474	7.2931	
$3s^{2}3p^{4}({}_{2}{}^{3}P)3d^{4}P$	$\frac{5}{2}$	7.44368	-0.0259	-0.0001	7.32474 7.41733	7.3868	
$3s^{2}3p^{4}(2^{3}P)3d^{4}F$	$\frac{3}{2}$ 7/2	7.50738	-0.0349	0.00018	7.41755	7.4433	
$3s^{2}3p^{4}({}_{2}{}^{1}D)3d^{2}P$	3/2	7.6436	-0.0351	0.00013	7.60879	7.5762	
$3s^{2}3p^{4}({}_{2}{}^{1}D)3d^{2}D$	$\frac{5}{2}$			0.00027			
$3s^{2}3p^{4}({}_{2}{}^{1}D)3d^{2}G$,	7.71975 7.74031	-0.0352		7.68483	7.6521	
3s ² 3p ⁴ (₂ ¹ D)3d ² G	7/2		-0.0334	0.0003	7.70725	7.676	
	9/2	7.83935	-0.0425	0.00033	7.79717	7.7673	
$3s^23p^4({}_2 {}^3P)3d {}^2F$	5/2	7.85615	-0.0332	0.00023	7.82313	7.7912	
$3s^{2}3p^{4}({}_{2}{}^{1}D)3d^{2}F$	5/2	8.15484	-0.0309	4.2E-05	8.12398	8.0883	
$3s^{2}3p^{4}({}_{2}{}^{1}D)3d^{2}F$	7/2	8.36445	-0.038	0.0002	8.32666	8.2913	
$3s^{2}3p^{4}(_{0} {}^{1}S)3d {}^{2}D$	3/2	8.68249	-0.0313	0.00013	8.65136	8.623	
$3s^23p^4({}_2 {}^1D)3d {}^2S$	1/2	8.98813	-0.0221	-0.0036	8.96243	8.9267	8.845
$3s^2 3p^4 (_0 {}^1S) 3d {}^2D$	5/2	9.09937	-0.0452	0.00064	9.05481	9.028	
$3s^23p^4({}_2{}^3P)3d {}^2P$	3/2	9.30401	-0.0278	4.2E-05	9.27627	9.2426	9.144
$3s^23p^4({}_2{}^3P)3d {}^2D$	5/2	9.35195	-0.0292	-0.0001	9.3226	9.2853	9.190
$3s^23p^4(2^{3}P)3d^{2}P$	1/2	9.60246	-0.0341	0.00019	9.56859	9.5356	9.436
$3s^23p^4({}_2{}^3P)3d {}^2D$	3/2	10.0608	-0.0422	0.00076	10.0193	9.9832	9.884
3s3p ⁵ (³ P)3d ⁴ P	1/2	11.2793	-0.0142	-0.0129	11.2522	11.219	
3s3p ⁵ (³ P)3d ⁴ P	3/2	11.3924	-0.0198	-0.0128	11.3598	11.327	
3s3p ⁵ (³ P)3d ⁴ P	5/2	11.6071	-0.0265	-0.0125	11.5681	11.534	
3s3p ⁵ (³ P)3d ⁴ F	9/2	11.8797	-0.0275	-0.0134	11.8388	11.804	
3s3p ⁵ (³ P)3d ⁴ F	7/2	11.9012	-0.0219	-0.0131	11.8662	11.829	
3s3p ⁵ (³ P)3d ⁴ F	5/2	12.0187	-0.0209	-0.0128	11.985	11.947	
3s3p ⁵ (³ P)3d ⁴ F	3/2	12.1621	-0.0209	-0.0126	12.1287	12.09	
3s3p ⁵ (³ P)3d ⁴ D	1/2	12.3641	-0.0179	-0.0109	12.3352	12.287	
$3s3p^{5}(^{3}P)3d^{4}D$	7/2	12.3891	-0.0256	-0.0124	12.351	12.308	
$3s3p^{5}(^{3}P)3d^{2}D$	5/2	12.5029	-0.0234	-0.0116	12.4679	12.422	
$3s3p^{5}(^{3}P)3d^{2}F$	7'/2	12.5453	-0.0301	-0.0115	12.5038	12.46	
$3s3p^{5}(^{3}P)3d^{4}D$	3/2	12.554	-0.027	-0.0109	12.5161	12.471	
$3s3p^{5}(^{3}P)3d^{2}F$	5/2	12.6397	-0.0288	-0.0117	12.5992	12.554	
$3s3p^{5}(^{3}P)3d^{2}D$	3/2	12.6971	-0.0255	-0.0114	12.6602	12.611	
$3s3p^{5}(^{1}P)3d^{2}P$	1/2	12.8231	-0.0254	-0.0105	12.7872	12.733	
$3s^23p^3(_3 {}^4S)3d^2(_2 {}^3F)^6F$	5/2	13.0261	-0.0374	-0.003	12.9857	12.91	
$3s^{2}3p^{3}(_{3}{}^{4}S)3d^{2}(_{2}{}^{3}F)^{6}F$	$\frac{3}{2}$	13.0284	-0.0346	-0.003	12.9917	12.914	

Table 2. Energies (in Ryd.) of lowest 100 relativistic levels of Kr XX by MCDF method and comparison with FAC and NIST values.

(Table Contd.)

Label	J		MC	DF2		FAC	NIST
		DC	Breit	QED	Total		
$3s^23p^3(_3{}^4S)3d^2(_2{}^3F){}^6F$	1/2	13.0446	-0.035	-0.002	13.0077	12.931	
$3s^23p^3(_3^4S)3d^2(_2^3F)$ ⁶ F	7/2	13.0582	-0.0422	-0.0013	13.0147	12.935	
$3s3p^{5}(^{3}P)3d^{2}F$	5/2	13.065	-0.0355	-0.0097	13.0197	12.97	
$3s^{2}3p^{3}({}_{3}{}^{4}S)3d^{2}({}_{2}{}^{3}F)^{6}F$	9'/2	13.1147	-0.0485	-0.001	13.0652	12.985	
$3s^23p^3(_3 {}^4S)3d^2(_2 {}^3F) {}^6F$	11/2	13.1773	-0.0559	-0.0009	13.1206	13.04	
3s3p ⁵ (¹ P)3d ² P	3/2	13.2917	-0.0365	-0.0094	13.2458	13.189	
$3s3p^5(^1P)3d ^2F$	5/2	13.3835	-0.035	-0.0079	13.3406	13.279	
$3s^23p^3(3^4S)3d^2(2^3P)^6P$	3/2	13.4112	-0.0374	-0.0012	13.3726	13.299	
$3s^23p^3(_3 {}^4S)3d^2(_2 {}^3P) {}^6P$	7/2	13.4348	-0.0435	-0.0014	13.3899	13.317	
$3s^23p^3(_3 {}^4S)3d^2(_2 {}^3P) {}^6P$	5/2	13.4577	-0.0404	-0.0013	13.416	13.343	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3P){}^4F$	3/2	13.5615	-0.0325	-0.0024	13.5266	13.446	
$3s^23p^3(^1P)3d^2F$	7/2	13.6037	-0.0427	-0.0072	13.5537	13.489	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3P){}^4P$	1/2	13.6351	-0.0367	-0.0014	13.5969	13.515	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^4G$	5/2	13.7122	-0.0396	-0.002	13.6706	13.588	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F) {}^4G$	7/2	13.7611	-0.0431	-0.0017	13.7162	13.635	
$3s3p^{5}(^{1}P)3d^{2}D$	3/2	13.807	-0.0325	-0.0017	13.7668	13.695	
$3s^23p^3(_3{}^4S)3d^2(_2{}^1D){}^4D$	$\frac{5}{2}$	13.8426	-0.0325	-0.0017	13.7003 13.7971	13.095 13.716	
$3s^{2}3p^{3}({}_{3}{}^{4}S)3d^{2}({}_{2}{}^{1}D)^{4}D$	$\frac{5}{2}$ 7/2	13.8420 13.8648	-0.044 -0.0442	-0.0013	13.7971	13.710 13.737	
$3s^{2}3p^{3}({}_{3}{}^{4}S)3d^{2}({}_{2}{}^{1}D)^{4}D$	3/2	13.8048 13.8736	-0.0442	-0.0021	13.8105 13.8301	13.757 13.753	
$3s3p^{5}(^{1}P)3d^{2}D$	$\frac{5}{2}$	13.9351	-0.0421	-0.0014	13.8301 13.8874	13.755 13.815	
$3s^23p^3(_3{}^4S)3d^2(_2{}^1D){}^4D$	$\frac{5/2}{1/2}$		-0.0408	-0.0071			
$3s^{2}3p^{3}(_{3}^{2}D)3d^{2}(_{2}^{3}P)^{4}P$	$\frac{1}{2}$ 5/2	13.9427 13.9834	-0.0441 -0.0416	-0.0012	$13.8974 \\ 13.9407$	$13.822 \\ 13.851$	
$3s^{2}3p^{3}(_{3}{}^{2}D)3d^{2}(_{2}{}^{3}F)^{4}H$							
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}P) {}^{4}P$	7/2	13.9845	-0.0457	-0.0016	13.9372	13.855	
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}F) {}^{4}G$	3/2	13.9899	-0.047	-0.0008	13.9421	13.855	
$3s^{2}3p^{3}(_{3}^{2}D)3d^{2}(_{2}^{3}F)$ ⁴ H	9/2	13.9964	-0.0518	-0.0008	13.9438	13.861	
	9/2	14.0478	-0.0443	-0.0011	14.0025	13.911	
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}F) {}^{4}G$	$\frac{11}{2}$	14.0868	-0.0555	-0.0008	14.0305	13.942	
$3s^{2}3p^{3}(_{3}{}^{4}S)3d^{2}(_{2}{}^{3}P) {}^{4}P$	5/2	14.124	-0.05	-0.0008	14.0733	13.99	
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}P) {}^{4}F$	7/2	14.1953	-0.0525	-0.0005	14.1423	14.056	
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}F)^{4}H$	11/2	14.2722	-0.0569	-0.0006	14.2146	14.121	
$3s^{2}3p^{3}({}_{3}{}^{2}D)3d^{2}({}_{2}{}^{3}P) {}^{4}F$	9/2	14.3258	-0.0573	-0.0004	14.2681	14.179	
$3s^{2}3p^{3}(_{3}{}^{2}D)3d^{2}(_{2}{}^{1}D){}^{2}D$	3/2	14.3424	-0.0396	-0.0022	14.3005	14.213	
$3s^{2}3p^{3}(_{3}{}^{2}D)3d^{2}(_{2}{}^{3}F){}^{2}H$	9/2	14.357	-0.0519	-0.0006	14.3046	14.222	
$3s^23p^3(_3{}^2D)3d^2(_2{}^1D){}^2F$	5/2	14.3587	-0.0425	-0.0018	14.3145	14.234	
$3s^23p^3(_3{}^2D)3d^2(_2{}^1D){}^2F$	7/2	14.4029	-0.0528	-0.0011	14.349	14.266	
$3s3p^5(^{3}P)3d^{2}P$	1/2	14.4131	-0.0318	-0.0082	14.3731	14.303	
3s3p ⁵ (³ P)3d ² P	3/2	14.497	-0.0358	-0.0086	14.4526	14.356	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^4H$	13/2	14.5222	-0.0683	-0.0004	14.4536	14.372	
3s ² 3p ³ (3 ² D)3d ² (2 ³ F) ² H	11/2	14.527	-0.0603	-0.0004	14.4663	14.386	
$3s^23p^3(_1{}^2P)3d^2(_2{}^3F){}^4G$	7/2	14.5383	-0.0449	-0.0013	14.4921	14.407	
$3s^23p^3(_1{}^2P)3d^2(_2{}^3F){}^4G$	5/2	14.5795	-0.0435	-0.0021	14.5339	14.452	
$3s^{2}3p^{3}(_{3}{}^{2}D)3d^{2}(_{2}{}^{1}D){}^{2}D$	5/2	14.6175	-0.0478	-0.0014	14.5683	14.483	
$3s^23p^3(_3{}^2D)3d^2(_2{}^1D){}^2G$	7/2	14.6984	-0.0481	-0.0014	14.6489	14.562	
$3s^23p^3(_3{}^2D)3d^2(_2{}^1D){}^2G$	9/2	14.7581	-0.0566	-0.0007	14.7008	14.614	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^4F$	5/2	14.7788	-0.0451	-0.0024	14.7313	14.651	
$3s^23p^3(_1{}^2P)3d^2(_2{}^3F){}^4D$	1/2	14.8168	-0.0358	-0.0027	14.7783	14.688	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F){}^4F$	3/2	14.8194	-0.044	-0.0023	14.7731	14.691	
$3s^23p^3(_3^4S)3d^2(_2^1G)^4G$	7/2	14.8217	-0.0483	-0.0011	14.7723	14.695	
$3s^23p^3(_3^2D)3d^2(_2^3P)^4P$	3/2	14.8377	-0.0327	-0.0027	14.8023	14.715	
$3s^23p^3(_3{}^2D)3d^2(_2{}^3F)^4F$	9/2	14.8885	-0.0582	-0.0008	14.8295	14.742	
$3s^23p^3(_3^2D)3d^2(_2^1G)^2I$	11/2	14.9334	-0.0407	-0.0017	14.891	14.783	
$3s^23p^3(_3^4S)3d^2(_0^1S)^4S$	3/2	14.9346	-0.0499	-0.001	14.8837	14.809	

	2J	λ (in Å)	λ (in Å)	$A_{ji}(s-1)$	$A_{ji}(s-1)$	f _{ij}	f _{ij}	$S_{ij}(au)$	$S_{ij}(au)$	Vel/len
i	K	(b)NIST	(MCDF)	(Ref. [10])	(MCDF)	(Ref. [10])	(Ref. [10])			
1	3	1.76E+02	$1.73\text{E}+02^a$	9.34E+09	1.23E+10	2.18E-02	2.78E-02	5.06E-02	6.34E-02	9.40E-01
1	4	1.43E+02	$1.36\text{E}+02^a$	3.96E+07	2.78E+08	1.82E-04	3.88E-04	3.43E-04	6.97E-04	1.20E+00
1	5	1.42E+02	$1.38\mathrm{E}{+}02^{a}$	8.89E+07	8.29E+07	2.71E-04	2.38E-04	5.08E-04	4.34E-04	9.40E-01
1	7	1.40E+02		2.45E+08		3.61E-04		6.67E-04		9.00E-01
1	10	1.29E+02		1.10E+09		2.75E-03		4.69E-03		9.50E-01
1	11	1.29E+02	$1.26\text{E}+02^a$	2.35E+07	5.28E+07	2.94 E- 05	6.29 E- 05	5.01E-05	1.04E-05	1.60E+00
1	12	1.27E+02	$1.24\text{E}+02^a$	6.76E+09	6.42E+09	8.19E-03	7.45E-03	1.37E-02	1.22E-02	1.00E+00
1	13	1.26E+02	$1.22\text{E+}02^{a}$	1.89E+09	1.61E+09	6.74E-03	5.41E-03	1.12E-02	8.72E-03	1.10E+00
1	14	1.25E+02	$1.21\text{E}+02^a$	1.22E+09	4.28E+09	2.87E-03	9.55E-04	4.72E-03	1.54E-03	9.50E-01
1	15	1.24E+02	$1.21\text{E}+02^a$	2.41E+09	2.14E+09	5.60E-03	4.72E-03	9.18E-03	7.55E-03	1.10E+00
1	16	1.23E+02	$1.19\mathrm{E}{+}02^{a}$	1.19E+09	1.00E+09	4.03E-03	3.24E-03	6.52E-03	5.13E-03	1.00E+00
1	18	1.20E+02		2.03E+08		4.36E-04		6.87E-04		8.00E-01
1	19	1.19E+02	$1.15\mathrm{E}{+}02^{a}$	1.21E+09	9.51E+08	3.84E-03	2.87E-03	5.99E-03	4.39E-03	1.00E+00
1	22	1.16E+02	$1.13\text{E+}02^{a}$	9.30E+08	6.25E+08	2.84E-03	1.82E-03	4.35E-03	2.72E-03	1.10E+00
1	23	1.12E+02	$1.09\text{E+}02^{a}$	1.93E+09	1.64E+09	5.45E-03	4.45E-03	8.05E-03	6.44E-03	1.10E+00
1	25	1.05E+02		1.90E+10		3.16E-02		4.39E-02		1.00E+00
1	26	1.02E+02	$0.99\mathrm{E}+02^{a}$	3.12E+11	3.13E+11	2.42E-01	2.31E-01	3.23E-01	3.03E-01	1.00E+00
			$1.03\mathrm{E}{+}02^{b}$							
1	27	1.01E+02	$1.02\text{E}+02^a$	2.24E+10	1.12E+10	5.10E-02	1.78E-02	6.75E-02	2.36E-02	1.10E+00
1	28	9.82E+01	$9.96\mathrm{E}{+}01^b$	2.89E+11		4.17E-01		5.40E-01		1.00E+00
			$0.99\mathrm{E}{+}02^{b}$							
1	29	9.77E+01	$9.43\text{E}+01^a$	3.27E+11	3.79E+11	7.03E-01	7.59E-01	9.05E-01	9.43E-01	1.10E+00
1	30	9.52E+01	$9.15\text{E}+01^a$	3.87E+10	5.81E+10	2.63E-02	3.65 E-02	3.30E-02	4.40E-02	9.90E-01
1	31	9.10E+01	$8.77\text{E}+01^a$	1.62E+09	1.15E+09	2.01E-03	1.33E-03	2.41E-03	1.52E-03	1.30E+00

Table 3. Transition data for E1 transitions from $3s^2 3p^5 {}^2P_{\frac{3}{2}}$: levels and 2J for ower level *I*, upper level *k*, wavelength λ (in Å), line strength *S*(length form), oscillator strength *f* (length form), transition rate A_{ji} (length form). Last column represents ratio of vel. and len. form of oscillator strength (Cl-like Kr)

^{*a*} Ref. [10] ^{*b*} Ref. [42]

The fundamental criteria to judge the accuracy of calculated radiative data's is the agreement between length and velocity form of radiative data. Therefore vel/len ratios of results of absorption oscillator strength are listed in last column of Table 3. The difference between both forms for strong El strong transformation ($f \ge 0.1$) does not exceed 10%. The ratio can be larger for same weak transition (f < 0.1). This is due to mixing present in there levels with the other levels. Additionally because their energy is very small hence slight variation in ΔE has a considerable effect on radiative rates.

Level		λ (in Å)	$A_{ji}(s-1)$	f_{ij}	$S_{ij}(au)$
i	j	-			
1	3	1.76E+02	3.32E+02	7.74E-10	7.60E+00
1	4	1.43E+02	6.62E+00	3.04E-11	1.59E-01
1	5	1.42E+02	1.24E+00	3.78E-12	1.96E-02
1	6	1.41E+02	3.78E+02	2.26E-09	1.14E+01
1	7	1.40E+02	2.04E+02	3.00E-10	1.48E+00
1	9	1.32E+02	1.25E+02	6.53E-10	2.69E+00
1	10	1.29E+02	1.22E+02	3.07E-10	1.19E+00
1	11	1.29E+02	3.79E+02	4.75E-10	1.84E+00
1	12	1.27E+02	1.13E+02	1.37E-10	5.05E-01
1	13	1.26E+02	3.79E+01	1.35E-10	4.80E-01
1	14	1.25E+02	2.24E+00	5.24E-12	1.83E-02
1	15	1.24E+02	9.89E+01	2.29E-10	7.91E-01
1	16	1.23E+02	3.74E+02	1.27E-09	4.22E+00
1	17	1.22E+02	1.07E+00	4.79E-12	1.55E-02
1	18	1.20E+02	1.03E+02	2.22E-10	6.82E-01
1	19	1.19E+02	2.08E+01	$6.57 \text{E}{-}11$	1.96E-01
1	20	1.18E+02	5.14E+01	2.15E-10	6.37E-01
1	22	1.16E+02	1.34E+01	4.08E-11	1.15E-01
1	23	1.12E+02	5.29E+01	1.50E-10	3.78E-01
1	24	1.09E+02	4.30E-01	1.54E-12	3.62E-03
1	25	1.05E+02	2.58E+02	4.30E-10	8.99E-01
1	26	1.02E+02	1.21E+01	9.40E-12	1.77E-02
1	27	1.01E+02	7.70E+01	1.75E-10	3.20E-01
1	28	9.82E+01	2.64E+02	3.82E-10	6.47E-01
1	29	9.77E+01	1.58E+01	3.39E-11	5.66E-02
1	30	9.52E+01	2.06E+00	1.40E-12	2.17E-03

Table 4. Transition data for M2 transitions from $3s^2 3p^5 2P_{3/2}$ levels and 2J for lower level *i*, upper level *k*, wavelength λ (in Å), line strength *S* (length form), oscillator strength *f* (length form), transition rate A_{ii} (length form), (Cl-like Kr).

4. Lifetimes

The lifetime τ of a level *j* can be obtained from the reciprocal of the sum of transition probabilities of radiative transitions from level *i* as

$$\tau_j(s) = \frac{1}{\sum_i A_{ji}(s^{-1})}.$$
(4.1)

Journal of Atomic, Molecular, Condensate & Nano Physics, Vol. 3, No. 2, pp. 137–150, 2016

In Table 1, lifetimes for lowest 100 fine-structure levels of Kr XX calculated by including all E1 (electric dipole), M1 (magnetic dipole), E2 (electric quadrupole) and M2 (magnetic quadrupole) transitions has been listed. As there are no comparisons for lifetimes in the literature, i believe that lifetimes reported by us for higher levels in the present paper will be helpful for future comparisons.

5. Conclusion

Motivated by the need of reliable and large amount of atomic data, energy levels, lifetimes and radiative data for lowest 100 fine structure-levels belonging to the configurations $3s^23p^5$, $3s3p^6$, $3s^23p^43d$, $3s3p^53d$ and $3s^23p^33d^2$ for Kr XX have presented. MCDF method have been used for present calculations included the contribution of QED and Breit corrections. MCDF energies are in good agreement with other available results and also the ratio of vel/len. ensures the authenticity and reliability of presented results. Conclusively, work in the present paper is comprehensive and consistent and may be beneficial in the examination of new data from fusion devices and astrophysical sources and in the modeling and characterization of plasma.

References

- J.E. Rice, K.B. Fournier, J.A. Goetz, E.S. Marmar and J.L. Terry, X-ray observations of 2*l*-n*l*['] transitions and configuration-interaction effects from Kr, Mo, Nb and Zr in near neon-like charge states from tokamak plasmas, *J. Phys. B* **33** (2000), 5435.
- [2] C. Jupen, B. Denne and I. Martinson, Transitions in Al-like, Mg-like and Na-like Kr and Mo, observed in the JET Tokamak, *Phys. Scr.* **41** (1990), 669.
- [3] S.O. Dean, Fusion and Energy Policy S. O Dean, J. Fusion Energy 25 (2006), 35.
- [4] N. Verma, A.K.S. Jha and M. Mohan, Transitions in Co XI, J. Phys. B 38 (2005), 3185.
- [5] E. Biemont and E. Trabert, Transition rates of the resonance line doublet in the Cl I sequence, Ar II-Ge XVI, J. Phys. B 33 (2000), 2939.
- [6] N.J. Wilson, A. Hibbert and K.L. Bell, Oscillator Strengths for K III, Ca IV and Sc V, Phys. Scr. 61 (2000), 603.
- [7] M. Mohan and A. Hibbert, Level energies and oscillator strengths in Cu XIII, J. Phys. B 25 (1992), 4427.
- [8] S. Aggarwal, J. Singh, A.K.S. Jha and M. Mohan, Photoionization Cross-section of Chlorine-like Iron, Jr. Astrophys. Astron. 33 (2012), 291.
- [9] A.K. Bhatia and G.A. Doschek, Atomic Data and Spectral Line Intensities for C-Like Mg VII, At. Data Nucl. Data Tables 60 (1995), 97.
- [10] K.N. Huang, Y.K. Kim and K.T. Cheng, Energy-level scheme and transition probabilities of Cl-like ions, At. Data Nucl. Data Tables 28 (1983), 355
- [11] B.C. Fawcett, Improved oscillator strength calculations for Ti VI and Fe X, At. Data Nucl. Data Tables, 47 (1991), 319.
- [12] K.A. Berrington, J.C. Pelan and J.A. Waldock, Oscillator strength for 3s23p5-3s3p6 in Cl-like ions, J. Phys. B 34 (2001), L419.

- [13] P.D. Dumont, H.P. Gornir, Y. Baudinet-Robinet and Kapenyak, Lifetime Measurements in Ti IV-VII Using Transitions Observed in Beam-Foil Spectroscopy between 400 and 800Å, J. Opt. Soc. Am. 71 (1981), 502.
- [14] A.E. Livington, D.J.G. Irwin and E.H. Pinnington, Lifetime measurements in Ar II-Ar VIII, J. Opt. Soc. Am. 62 (1972), 1303.
- [15] E. Trabert, Experimental checks on calculations for Cl-, S- and P-like ions of the iron group elements, *J. Phys. B* 29 (1996), L217.
- [16] V. Kaufman, J. Sugar and W.L. Rowan, Chlorine like spectra of copper to molybednum, J. Opt. Soc. Am. B 6 (1989), 1444.
- [17] G.C. Rodrigues, P. Indelicato, J.P. Santos, P. Patte and F. Parente, Systematic calculation of total atomic energies of ground state configurations, *At. Data Nucl. Data Tables* **86** (2004), 117.
- [18] E.B. Saloman, Energy Levels and Observed Spectral Lines of Krypton, Kr I through Kr XXXVI, J. Phys. Chem. Ref. Data 36 (2007), 215.
- [19] K.L. Baluja and A. Agrawal, M1 Transition probabilities between Five Structure components ${}^{2}L_{J}$ (L > 1), Z. Phys. D 33 (1995), 167.
- [20] R.L. Kelly, Erratum: Atomic and Ionic Spectrum Lines below 2000 Angstroms: Hydrogen through Krypton, Part III (Finding List) [J. Phys. Chem. Ref. Data 16, Suppl. 1 (1987)], J. Phys. Chem. Ref. Data 16 (1987), Suppl.1 1.
- [21] J. Sugar and A. Musgrove, Energy Levels of Krypton, Kr I through Kr XXXVI, J. Phys. Chem. Ref. Data 20 (5) 1991), 859.
- [22] V. Kaufman and J. Sugar, Forbidden Lines in ns^2np^k ground configurations and nsnp excited configuration of beryllium through molybdenum atoms and ions, *J. Phys. Chem. Ref. Data* **15** (1) 1986), 321.
- [23] E. Biemont, Y. Fremat and P. Quinet, Ionization potentials of atoms and ions from lithium to tin (z = 50), At. Data Nucl. Data Tables 71 (1999), 117.
- [24] T.A. Carlson, C.W. Nestor Jr., N. Wasserman and J.D. McDowell, Calculated ionization potentials for multiply charged ions, *Atomic Data* 2 (1970), 63.
- [25] R.L. Kelly and D.E. Harrison Jr, Ionization Potential, experimental and theoretical of the elements hydrogen to krypton, At. Data Nucl. Data Tables 3 (1971), 177.
- [26] M.V. Samii and K. MacDonald, Electric dipole transitions in CL-like ions, At. Data Nucl. Data Tables 26 (1981), 467.
- [27] J.F. Wyart and TFR group, Identification of Krypton Kr XVIII to Kr XXIX Spectra Excited in TFR Tokamak Plasmas, *Phys Scr.* 31 (1985), 539.
- [28] B. Denne, E. Hinnov, S. Suckewer and S. Cohen, Magnetic Dipole Lines in the $3s^23p^x$ configurations of elements from copper to Molybednum, *Physical review A* 28 (1) (1983), 206.
- [29] J.R. Roberts, T.L. Pittman, J. Sugar, V. Kaufman and W.L. Rowan, Magnetic-Dipole wavelength measurements in the n = 3 configurations of highly ionized Cu, Zn, Ga, As, Kr and Y, *Physical Review A* 35 (6) (1987), 2591.
- [30] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers and N.C. Pyper, An Atomic multiconfigurations Dirac-Fock package, *Comput Phys. Commun.* 21 (1980), 207.
- [31] K.G. Dyall, I.P. Grant, C.T. Johnson and E.P. Plummer, GRASP: a general purpose relativistic atomic structure program, *Comput. Phys. Commun.* 55 (1989), 425

- [32] F.A. Parpia, C.F. Fischer and I.P. Grant, GRASP92: A package for large-scaler relativistic atomic structure program, *Comput. Phys. Commun.* 94 (1996), 249.
- [33] P. Jonsson, X. He, C.F. Fischer and I.P. Grant, The grasp2k relativistic atomic structure package, Comput. Phys. Commun. 177 (2007), 597.
- [34] P.H. Norrington, http://www.am.qub.ac.uk/DARC/ (2009).
- [35] S. Aggarwal, J. Singh and M. Mohan, New atomic data for krXXXV useful in fusion plasma, *Chin. Phys. B* 22 (2013), 033201.
- [36] A.K. Singh, S. Aggarwal and M. Mohan, Level energies. Lifetimes and radiative rates in the $4p^44d$ configurations of Bromine-like ions, *Phys. Scr.* 88 (2013), 035301.
- [37] S. Aggarwal, J. Singh and M. Mohan, Breit–Pauli atomic structure calculations for Fe XI, At. Data Nucl. Data Tables 99 (2013), 704.
- [38] S. Aggarwal, A.K.S. Jha and M. Mohan, Multiconfigurational Dirac-Fock energy levels and radiative rates for Br-like Tungsten, *Can. J. Phys.* **91** (2013), 394.
- [39] M. Mohan, S. Aggarwal and N. Singh, Atomic data for F-like Tungsten, Can. J. Phys. 92 (2014), 177.
- [40] M. Mohan, S. Aggarwal, N. Singh and A.K.S. Jha, Reply to Comment on "Multiconfigural Dirac-Fock energy levels and radiative rates for Br-like Tungsten (*Can. J. Phys.* 91 (2013), 394)", *Can. J. Phys.* 92 (2014), 551.
- [41] S. Aggarwal, J. Singh, A.K.S. Jha and M. Mohan, Energy levels and radiative transition rates for Ge XXXI, As XXXII, and Se XXXIII, At. Data Nucl. Data Tables 100 (2014), 859.
- [42] http://www.nist.gov/pml/data/asd.cfm