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Lifetime calculations in energy levels of Kr VII

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Abstract

Calculations of the lifetimes for all experimentally known energy levels of the spectrum of the six times-ionized krypton (Kr VII) are presented. The relativistic Hartree–Fock method including core-polarization effects were used. The energy matrix was calculated using energy parameters adjusted to the experimental energy levels. We also present a calculation based on a relativistic multiconfigurational Dirac–Fock approach. For some energy levels, a comparison of these results with the bibliography data was made.

1. Introduction

Six times ionized krypton (Kr VII) belongs to the Zn I isoelectronic sequence. The analysis of the atomic structure of this ion is important in astrophysical plasma research and recently Kr VI and Kr VII lines have been observed in the ultraviolet spectrum of the hot DO-type white dwarf RE 0503-289 [1], in the first detection of krypton in this kind of star. Reliable measurements and calculations of atomic data are a prerequisite for state-of-the-art non-local thermodynamic equilibrium stellar-atmosphere modeling (NLTE). Observed Kr V–VII line profiles in the UV spectrum of the white dwarf RE 0503−289 were simultaneously well reproduced with newly calculated oscillator strengths [2]. The energy levels measured by Raineri *et al* [3] were used to fit the parameters of $4s^2$, $4p^2$, 4s4d, 4s5d, 4s6d, 4s5s, 4s6s, 4p4f, 4s4p, 4s5p, 4s6p, 4s4f, 4s5f, 4s6f, 4p5s, and 4p4d configurations in Kr VII. In that work, the spectrum was recorded in the 300–4800 Å wavelength range, resulting in 115 new classified lines and extended the analysis to 38 new energy levels belonging to 4s5s, 4s6s, 4p4f, 4s6d and 4p4d, 4s5p, 4s4f, 4p5s, 4s5f, 4s6p, 4s6f even and odd configurations, respectively. The authors also mentioned several discrepancies between the values on Kr VII published in papers by Churilov [4], Raineri *et al* [5] and Cavalcanti *et al* [6]. In order to clarify these disagreements they presented a new revised and extended analysis for the Kr VII. A critical compilation of the energy levels and transitions of the Kr VII ion was reported by Saloman [7]. Liang *et al* [8] presented calculations of line strengths, oscillator strengths, radiative decay rates and fine structure collision strengths for 90 lines in Kr VII. In their calculations, using the AUTOSTRUCTURE code [9], they included nine configurations, i.e., $4s^2$, $4p^2$, 4s4d, 4s5s, 4s5d, and 4s4p, 4s4f,4p4d, 4s5p for the even and odd parities, respectively.

Lifetimes depend on the allowed and forbidden transition probabilities from the corresponding states. The only experimental results for lifetimes of energy levels for Kr VII was provided by Pinnington *et al* [10, 11], who used the beam-foil method. They describe two techniques in their methods; from multiexponential curve fitting (d and f in in table 1) and from the arbitrarily normalized decay curve (ANDC) (e and g in table 1) where quoted errors are standard deviations. Empirical predictions are reported for the lifetimes of the $4s^2$–4s4p resonance and intercombination transitions in the Zn isoelectronic sequence [12]. Using configuration interaction wave functions, Hibbert *et al* [13] presented lifetime calculations of the 4s4p $^3P_1^0$ energy level in Kr VII. This value is in excellent agreement with the experiment. They also included core polarization (CP) effects in the calculation.

In the present work, we calculated the lifetimes for all experimentally known energy levels of the Kr VII [3, 7]. Four calculation methods were used to obtain the lifetimes of the energy levels. For the first three methods, Cowan's package [14] was used with corrections to the code made by Kramida [15], due to an error in Cowan's

atomic structure theory. The calculations were performed for different sets of configurations. We also included CP effects [16]. The fourth method is based on a multiconfigurational relativistic approach for the Dirac equation (MCDF), as described by Grant using the general relativistic atomic structure package (GRASP) [17]. For some levels we compared the lifetime values with experimental results [10, 11].

2. Theory

2.1. The Hartree–Fock (HF) method

In the codes rcn36/rcn2 of the Cowan program [14] the wavefunctions are calculated in a HF approximation with relativistic corrections (HFR). The wavefunctions are used to calculate a multiconfigurational energy matrix with the code rcg11. Both eigenvalues and eigenvectors of the matrix are functions of the Slater parameters, i.e., functions of the average configuration energy E_{av}, electrostatic direct F^k and exchange G^k integrals, effective radial parameter α, configuration interaction integrals R^k, and spin–orbit parameters ζ_{nl}. We had used this method in several previous papers for example [18, 19]. The values of these parameters were changed to fit the experimental values by means of a least-squares calculation. We also made the corrections proposed by Kramida [15] in the rcn2 code, in this way we obtained non-zero values for some configuration-interaction integrals of the Rydberg series, which were zero in the original version of rcn2.

The natural lifetime $\tau(\gamma J)$ is the inverse of transition probability, then:

$$\tau(\gamma J) = \left(\sum A(\gamma J, \gamma' J')\right)^{-1}, \tag{1}$$

where $A(\gamma J, \gamma' j')$ is obtained from equations (14.33) and (14.42) of [14].

2.2. HF plus CP

We included the CP effects (see, for example, Curtis [12] and Biémont *et al* [20]) just by replacing the dipole integral

$$\int_0^\infty P_{nl}(r) r P_{n'l'}(r)\,\mathrm{d}r \rightarrow \int_0^\infty P_{nl} r \cdot \left[1 - \frac{\alpha_d}{(r^2 + r_c^2)^{3/2}}\right] P_{n'l'}(r)\,\mathrm{d}r - \frac{\alpha_d}{r_c^3}\int_0^{r_c} P_{nl}(r) P_{n'l'}(r)\,\mathrm{d}r. \tag{2}$$

Here α_d is the electric dipole polarizability of the core, and r_c is the cut-off radius, which defines the boundaries of the atomic core. This is the same modification used by Quinet *et al* [21] to correct transition matrix elements when including CP effects. In our case, the radial functions were obtained from the single configuration HF method with relativistic corrections, and no modification was done to include CP effects in the Hamiltonian.

2.3. Relativistic Dirac–Fock calculations

The GRASP package solves the Dirac equations within the framework of relativistic quantum theory [17, 22]. This program offers energy levels, wavelength, dipole transition rates and lifetimes from a multiconfigurational relativistic approach. The configuration state functions are a linear combination of Slater determinants constructed from relativistic (Dirac) orbitals equation (4) of [18].

3. Results and discussions

The results of our four different lifetime calculations are presented in table 1. The experimental energy level values were taken from Raineri *et al* [3] and the experimental lifetimes from Pinnington *et al* [10, 11], who used the beam-foil method.

The HFR calculations were performed with different sets of configurations. In the first one (A), the following configurations were included: $4s^2$, $4p^2$, 4s4d, $4d^2$, 4s5s, 4s5d, 4p4f, $4f^2$, 4p5p, 4p5f, 4s6s, 4s6d, $3d^9 4s^2 4d$ and 4s4p, 4p4d, 4s5p, 4s4f, 4s5f, 4p5s, 4p5d, 4s6p, 4s6f, 4d4f, $3d^9 4s^2 4p$ for even and odd parity respectively, which is the same set used by Raineri *et al* [3]. The values of the adjusted parameters used in the present work are also similar to [3], where the details for the least-squares calculation are explained. The difference is that we considered the corrections made by Kramida [15] where we obtained non-zero values for some configuration-interaction integrals of Rydberg series (see point 2.1). These integrals were R^0(4s5d,4s6d), R^0(4s5p,4s6p) and R^0(4s5f,4s6f) with values in 605, 819, 458 cm^{-1}, respectively. The change in the electrostatic integrals is expected to be equivalent to the inclusion of electronic correlation effects of higher order in the final values of the energy levels.

Table 1. Lifetimes of Kr VII levels.

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
$4s^2\,{}^1S_0$	0.0	0.0	98	A	∞	
				B	∞	
				C	∞	
				D	∞	
$4s4p\,{}^3P_0$	117 389.6	117 399	100	A	∞	
				B	∞	
				C	∞	
				D	∞	
$4s4p\,{}^3P_1$	120 094.8	120 083	99	A	38.08	47 ± 10[d]
				B	45.03	
				C	42.04	
				D	65.75	
$4s4p\,{}^3P_2$	126 553.8	126 556	100	A	∞	
				B	∞	
				C	∞	
				D	∞	
$4s4p\,{}^1P_1$	170 835.0	170 835	97	A	0.088	0.101 ± 0.01[e]
				B	0.104	
				C	0.100	
				D	0.086	
$4p^2\,{}^3P_0$	274 931.7	274 906	96	A	0.108	0.158 ± 0.018[d]
				B	0.119	
				C	0.127	
				D	0.107	
$4p^2\,{}^3P_1$	279 414.5	279 449	100	A	0.102	0.156 ± 0.025[d]
				B	0.112	
				C	0.121	
				D	0.102	
$4p^2\,{}^3P_2$	288 190.2	288 172	$67\,4p^2\,{}^3P + 28\,4p^2\,{}^1D + 5\,4s4d\,{}^1D$	A	0.130	0.173 ± 0.015[d]
				B	0.144	
				C	0.155	
				D	0.343	
$4p^2\,{}^1D_2$	279 714.8	279 723	$59\,4p^2\,{}^1D + 32\,4p^2\,{}^3P + 8\,4s4d\,{}^1D$	A	0.240	0.081 ± 0.020[d]
				B	0.267	
				C	0.287	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.118	
$4p^2\ ^1S_0$	321 794.0	321 795	94	A	0.096	
				B	0.104	
				C	0.113	
				D	0.096	
$4s4d\ ^3D_1$	349 973.1	350 067	100	A	0.043	
				B	0.045	
				C	0.049	
				D	0.044	
$4s4d\ ^3D_2$	350 416.8	350 435	100	A	0.045	
				B	0.047	
				C	0.050	
				D	0.045	
$4s4d\ ^3D_3$	351 116.2	351 004	100	A	0.048	
				B	0.049	
				C	0.053	
				D	0.047	
$4s4d\ ^1D_2$	379 488.3	379 489	85 $4s4d\ ^1D$ + 13 $4p2\ ^1D$	A	0.033	0.046 ± 0.008[d]
				B	0.034	
				C	0.037	
				D	0.033	
$4s5s\ ^3S_1$	438 644	438 636	99	A	0.037	
				B	0.030	
				C	0.033	
				D	0.039	
$4s5s\ ^1S_0$	447 769	447 777	99	A	0.050	
				B	0.042	
				C	0.047	
				D	0.056	
$4p4d\ ^3F_2$	475 890	475 922	88 $4p4d\ ^3F$ + 7 $4p4d\ ^1D$ + 5 $4s4f\ ^3F$	A	0.527	
				B	0.643	
				C	0.644	
				D	0.725	
$4p4d\ ^3F_3$	479 655	479 663	92 $4p4d\ ^3F$ + 6 $4s4f\ ^3F$	A	0.720	
				B	0.898	
				C	0.902	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	1.005	
$4p4d\,^3F_4$	484 543	484 542	92 $4p4d\,^3F$ + 8 $4s4f\,^3F$	A	1.117	
				B	1.500	
				C	1.522	
				D	1.510	
$4p4d\,^1F_3$	505 076	505 016	36 $4p4d\,^1F$ + 34 $4s4f\,^1F$ + 29 $4p4d\,^3D$	A	0.035	
				B	0.039	
				C	0.039	
				D	0.029	
$4p4d\,^3D_1$	501 542	501 553	65 $4p4d\,^3D$ + 28 $4p4d\,^3P$	A	0.030	
				B	0.036	
				C	0.034	
				D	0.032	
$4p4d\,^3D_2$	507 934	507 873	62 $4p4d\,^3D$ + 36 $4p4d\,^3P$	A	0.030	
				B	0.034	
				C	0.034	
				D	0.037	
$4p4d\,^3D_3$	508 473	508 595	70 $4p4d\,^3D$ + 16 $4s4f\,^1F$ + 13 $4p4d\,^1F$	A	0.032	
				B	0.036	
				C	0.036	
				D	0.041	
$4p4d\,^1D_2$	487 650	487 605	87 $4p4d\,^1D$ + 6 $4p4d\,^3F$ + 5 $4p4d\,^3P$	A	0.066	
				B	0.076	
				C	0.076	
				D	0.067	
$4p4d\,^3P_0$	506 933	506 938	97	A	0.037	
				B	0.042	
				C	0.042	
				D	0.039	
$4p4d\,^3P_1$	507 446	507 448	66 $4p4d\,^3P$ + 32 $4p4d\,^3D$	A	0.033	
				B	0.037	
				C	0.037	
				D	0.034	
$4p4d\,^3P_2$	501 769	501 763	52 $4p4d\,^3P$ + 35 $4p4d\,^3D$ + 7 $4s5p\,^3P$	A	0.035	
				B	0.039	
				C	0.039	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.031	
$4p4d\ ^1P_1$	535 462	535 465	94	A	0.037	
				B	0.043	
				C	0.043	
				D	0.038	
$4s5p\ ^3P_0$	492 776	492 755	97	A	0.235	0.537 ± 0.040[f], 0.330 ± 0.040[g]
				B	0.224	
				C	0.225	
				D	0.250	
$4s5p\ ^3P_1$	493 219	493 242	86 $4s5p\ ^3P$ + 10 $4s5p\ ^1P$	A	0.209	0.497 ± 0.040[f], 0.305 ± 0.040[g]
				B	0.189	
				C	0.189	
				D	0.218	
$4s5p\ ^3P_2$	495 578.4	495 580	90 $4s5p\ ^3P$ + 7 $4p4d\ ^3P$	A	0.223	0.510 ± 0.030[f], 0.30 ± 0.08[g]
				B	0.217	
				C	0.219	
				D	0.234	
$4s5p\ ^1P_1$	497 395	497 392	84 $4s5p\ ^1P$ + 9 $4s5p\ ^3P$	A	0.097	0.289 ± 0.040[f]
				B	0.078	
				C	0.078	
				D	0.096	
$4s4f\ ^3F_2$	530 349	530 285	94 $4s4f\ ^3F$ + 6 $4p4d\ ^3F$	A	0.045	
				B	0.047	
				C	0.047	
				D	0.045	
$4s4f\ ^3F_3$	530 491	530 504	93 $4s4f\ ^3F$ + 7 $4p4d\ ^3F$	A	0.044	
				B	0.047	
				C	0.047	
				D	0.045	
$4s4f\ ^3F_4$	530 772	530 822	92 $4s4f\ ^3F$ + 8 $4p4d\ ^3F$	A	0.044	
				B	0.047	
				C	0.047	
				D	0.044	
$4s4f\ ^1F_3$	560 671	560 664	49 $4s4f\ ^1F$ +48 $4p4d\ ^1F$	A	0.024	
				B	0.026	
				C	0.026	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.024	
4s5d $^3D_1$	578 470	578 518	98	A	0.237	0.426 ± 0.030[f]
				B	0.241	
				C	0.250	
				D	0.253	
4s5d $^3D_2$	578 722	578 728	98	A	0.241	0.437 ± 0.030[f]
				B	0.245	
				C	0.254	
				D	0.255	
4s5d $^3D_3$	579 109	579 056	99	A	0.249	0.491 ± 0.050[f]
				B	0.255	
				C	0.262	
				D	0.263	
4s5d $^1D_2$	581 038	581 038	96	A	0.210	
				B	0.227	
				C	0.236	
				D	0.216	
4p5s $^3P_0$		585 764	99	A	0.051	
				B	0.049	
				C	0.049	
				D	0.050	
4p5s $^3P_1$	587 029	587 029	84 4p5s ^3P + 14 4p5s ^1P	A	0.045	
				B	0.042	
				C	0.043	
				D	0.046	
4p5s $^3P_2$	594 617	594 617	99	A	0.047	
				B	0.045	
				C	0.045	
				D	0.048	
4p5s $^1P_1$	598 281	598 281	79 4p5s ^1P + 15 4p5s ^3P	A	0.029	
				B	0.027	
				C	0.027	
				D	0.028	
4s6s $^3S_1$	616 314	616 314	99	A	0.055	
				B	0.046	
				C	0.047	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.052	
$4s6s\ ^1S_0$	618 693	618 693	98	A	0.064	
				B	0.056	
				C	0.061	
				D	0.072	
$4s5f\ ^3F_2$	656 725	656 803	99	A	0.203	
				B	0.212	
				C	0.213	
				D	0.220	
$4s5f\ ^3F_3$	656 868	656 845	99	A	0.203	
				B	0.212	
				C	0.213	
				D	0.222	
$4s5f\ ^3F_4$	656 956	656 901	99	A	0.203	
				B	0.213	
				C	0.214	
				D	0.223	
$4s5f\ ^1F_3$	659 927	659 919	96	A	0.177	
				B	0.187	
				C	0.188	
				D	0.170	
$4p4f\ ^3G_3$	671 908	671 921	$47\,4p4f\ ^3G + 31\,4p4f\ ^1F + 20\,4p4f\ ^3F$	A	0.049	
				B	0.048	
				C	0.054	
				D	0.049	
$4p4f\ ^3G_4$		673 646	$63\,4p4f\ ^3G + 24\,4p4f\ ^1G + 9\,4d^2\ ^1G$	A	0.070	
				B	0.067	
				C	0.078	
				D	0.057	
$4p4f\ ^3G_5$		671 786	100	A	0.050	
				B	0.047	
				C	0.053	
				D	0.050	
$4p4f\ ^1G_4$	671 378	671 351	$46\,4p4f\ ^3F + 30\,4p4f\ ^1G + 11\,4d^2\ ^1G$	A	0.094	
				B	0.093	
				C	0.106	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.118	
$4p4f\,^3F_2$	664 923	665 007	86 $4p4f\,^3F$ + 7 $4d^2\,^3F$	A	0.063	
				B	0.062	
				C	0.071	
				D	0.064	
$4p4f\,^3F_3$	664 997	664 897	49 $4p4f\,^3F$ + 38 $4p4f\,^1F$ + 9 $4p4f\,^3D$	A	0.054	
				B	0.053	
				C	0.059	
				D	0.049	
$4p4f\,^3F_4$	663 983	664 015	43 $4p4f\,^3F$ + 28 $4p4f\,^3G$ + 21 $4p4f\,^1G$	A	0.078	
				B	0.076	
				C	0.086	
				D	0.091	
$4p4f\,^1F_3$		663 879	53 $4p4f\,^3G$ + 27 $4p4f\,^1F$ + 19 $4p4f\,^3F$	A	0.051	
				B	0.049	
				C	0.056	
				D	0.049	
$4p4f\,^3D_1$	684 070	684 002	99	A	0.043	
				B	0.042	
				C	0.047	
				D	0.048	
$4p4f\,^3D_2$	681 681	681 336	65 $4p4f\,^3D$ + 23 $4p4f\,^1D$ + 6 $4p4f\,^3F$	A	0.046	
				B	0.045	
				C	0.050	
				D	0.049	
$4p4f\,^3D_3$	680 086	680 361	89 $4p4f\,^3D$ + 5 $4p4f\,^1F$ + 4 $4p4f\,^3F$	A	0.045	
				B	0.043	
				C	0.049	
				D	0.046	
$4p4f\,^1D_2$	684 941	685 081	54 $4p4f\,^1D$ + 31 $4p4f\,^3D$ + 13 $4d^2\,^1D$	A	0.046	
				B	0.046	
				C	0.050	
				D	0.055	
$4s6p\,^3P_0$	640 160	640 334	100	A	0.258	
				B	0.241	
				C	0.242	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.240	
4s6p $^3P_1$	640 761	640 780	97	A	0.251	
				B	0.231	
				C	0.232	
				D	0.233	
4s6p $^3P_2$	642 010	642 050	100	A	0.248	
				B	0.232	
				C	0.233	
				D	0.238	
4s6p $^1P_1$	645 430	645 423	94	A	0.140	
				B	0.104	
				C	0.105	
				D	0.130	
4s6d $^3D_1$	694 858	694 857	99	A	0.239	
				B	0.236	
				C	0.251	
				D	0.195	
4s6d $^3D_2$	695 056	694 957	99	A	0.242	
				B	0.240	
				C	0.255	
				D	0.217	
4s6d $^3D_3$	695 015	695 115	99	A	0.248	
				B	0.247	
				C	0.263	
				D	0.299	
4s6d $^1D_2$	697 330	697 330	94	A	0.205	
				B	0.192	
				C	0.207	
				D	0.128	
4s6f $^3F_2$	724 718	724 629	78 4s6f ^3F + 17 4p5d ^3F	A	0.273	
				B	0.303	
				C	0.305	
				D	0.160	
4s6f $^3F_3$	724 826	725 127	69 4s6f ^3F + 24 4p5d ^3F + 4p5d ^3D	A	0.233	
				B	0.260	
				C	0.259	

Table 1. (Continued.)

Designation	E_{exp} (cm^{-1})[a]	E_{cal} (cm^{-1})[b]	Percentage composition[c]	Type of calculation	Lifetime (ns)	Experimental lifetime (ns)
				D	0.432	
$4s6f\,^3F_4$	725 989	726 069	$59\,4s6f\,^3F + 40\,4p5d\,^3F$	A	0.189	
				B	0.210	
				C	0.205	
				D	0.454	
$4s6f\,^1F_3$	719 130	718 791	$42\,4s6f\,^1F + 22\,4p5d\,^1F + 15\,4p5d\,^3F$	A	0.359	
				B	0.411	
				C	0.306	
				D	0.235	

[a] Experimental energy level reported by Raineri [3].

[b] Calculated energy level values obtained using the fitted energy parameters [3].

[c] Percentages below 4% have been omitted [3].

[d, e] Experimental lifetimes reported by Pinnington [10].

[f, g] Experimental lifetimes reported by Pinnington [11].

A: Calculated HFR lifetimes values obtained using the fitted energy parameters obtained in [3].

B: Calculated HFR lifetimes values including core polarization effects (CP).

C: Calculated HFR lifetimes values including core polarization effects (CP) and the $5s^2 + 5p^2 + 5s5p$ configurations.

D: Calculated GRASP lifetimes values considering babuskin gauge and the configuration set used in C.

Table 2. Energy parameters (cm^{-1}) for the studied even parity configurations in the calculation C of Kr VII.

Configuration	Parameter	HF value	Fitted value	F/HF(a)
$4s^2$	E_{av}	0.0	7319 ± 158	
$4p^2$	E_{av}	281 386	290 937 ± 90	1.034
	$F^2(4p, 4p)$	71 534	61 457 ± 474	0.859
	α	0.0	7(FIX)	
	ζ_{4p}	5484	6021 ± 96	1.098
4s4d	E_{av}	346 026	356 442 ± 82	1.030
	ζ_{4d}	403	383 (FIX)	0.950
	$G^2(4s, 4d)$	53 495	47 443 ± 523	0.886
4s5s	E_{av}	432 198	442 930 ± 123	1.025
	$G^0(4s, 5s)$	6340	5311 ± 111	0.838
4s5d	E_{av}	571 300	581 207 ± 80	1.017
	ζ_{5d}	175	166 (FIX)	0.950
	$G^2(4s, 5d)$	11 272	9785 ± 469	0.868
4p4f	E_{av}	665 051	676 357 ± 75	1.017
	ζ_{4p}	5473	6521 ± 139	1.191
	ζ_{4f}	9	9 (FIX)	1.000
	$F^2(4p, 4f)$	45 588	44 142 ± 635	0.968
	$G^2(4p, 4f)$	37 759	41 680 ± 1006	1.104
	$G^4(4p, 4f)$	25 506	28 968 ± 918	1.136
4s6s	E_{av}	607 519	617 504 ± 125	1.016
	$G^0(4s, 6s)$	2141	1720 ± 113	0.803
4s6d	E_{av}	675 806	695 134 ± 79	1.028
	ζ_{6d}	91	87 (FIX)	0.950
	$G^2(4s, 6d)$	4632	3865 ± 463	0.834
Configuration interaction integrals				
4s4d–4f 4p	$R^1(4s4d, 4f4p)$	65 718	49 288 (FIX)	0.750
$5s^2$–$5p^2$	$R^1(5s5s, 5p5p)$	47 319	35 489(FIX)	0.750

Note. (a) Parameters omitted from this table: direct and exchange integrals, and spin–orbit parameters set for configurations that not have known experimental levels, this values were set to 85%, 85%, and 95% of their HFR values respectively; CI omitted integrals were set to 85% of their HFR values. The standard deviation for energy adjustment was 155 cm^{-1}.

The second calculation (B) is the same as the first one, except that in this case we did not consider core excited configuration, but instead, we took into account CP effects. This inclusion required the knowledge of the dipole polarizability of the ionic core, α_d, and of the cutoff radius, r_c. For the first parameter, we used the value computed by Fraga *et al* [23] for the Kr^{8+} ion, i.e. $\alpha_d = 0.209\ a_0^3$, while the cutoff radius, r_c, was chosen equal to 0.56, which corresponds to the mean HFR $\langle r \rangle$ value of the outermost core orbital $3d^{10}$.

The third calculation (C) is the same as the second one including CP effects except that we considered the valence shell correlation [13] taking into account $5s^2$, $5p^2$ and 5s5p configurations. The least-squares calculation results for the energy parameters are shown in tables 2 and 3 for the even and odd parities, respectively. For the even parity, all parameters (E_{av}, F^2, G^0, G^2, G^4 and spin–orbit) were left free for the known configurations. In order to reduce the standard deviation and to obtain parameter values in accordance with the scaled HF values, all the configuration–interaction integrals were scaled down at 85% of their HF values, except for the corresponding to 4s4d–4f 4p and $5s^2$–$5p^2$ that were held fixed at 75% of their HF values. For the odd parity, all parameters (E_{av}, F^2, G^1, G^3 and spin–orbit) were left free for the known configurations except for the G^3(4s,6f) that was held fixed at 85% of the HF value. The 4s4p–4p 4d interaction integral was held fixed at 75% of their HF values and those corresponding to 4p4d–4s4f were let free to optimize their values and then fixed for the final calculation. The standard deviation for the energy adjustment was 155 cm^{-1} and 158 cm^{-1} for the even and odd parities, respectively.

The fourth calculation (D) was the fully relativistic MCDF approach. We used the GRASP [17]. Computations were carried out with the extended average level assuming a uniform charge distribution in the nucleus, with a krypton atomic weight of 83.80. We considered the same numbers and type of configurations as in the C calculation. The values presented in this work for lifetimes are in Babushkin gauge since this one, in the non-relativistic limits (length), has been found to be the most stable value in many situations, in the sense that it

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

Configuration	Parameter	HF value	Fitted value	F/HF(a)
4s4p	E_{av}	127 325	137 895 + 87	1.083
	ζ_{4p}	5500	6130 ± 144	1.114
	G^1(4s, 4p)	93 862	79 316 ± 299	0.845
4p4d	E_{av}	490 335	502 378 ± 55	1.024
	ζ_{4p}	5601	6258 ± 120	1.117
	ζ_{4d}	413	392 (FIX)	0.950
	F^2(4p, 4d)	60 639	54 845 ± 513	0.904
	G^1(4p, 4d)	74 858	65 164 ± 273	0.870
	G^3(4p, 4d)	46 888	41 677 ± 455	0.889
4s5p	E_{av}	487 599	497 486 ± 94	1.020
	ζ_{5p}	1950	2055 ± 141	1.054
	G^1(4s, 5p)	9827	7661 ± 389	0.779
4s4f	E_{av}	518 166	528 984 ± 108	1.021
	ζ_{4f}	8	8 (FIX)	1.000
	G^3(4s, 4f)	26 286	22 919 ± 1208	0.872
4s5f	E_{av}	646 259	658 081 ± 81	1.018
	ζ_{5f}	5	5 (FIX)	1.000
	G^3(4s,5f)	10 763	10 392 ± 663	0.965
4p5s	E_{av}	581 531	592 396 ± 95	1.019
	ζ_{4p}	5803	5938 ± 149	1.023
	G^1(4p, 5s)	9110	6550 ± 407	0.719
4s6p	E_{av}	634 019	641 988 ± 87	1.012
	ζ_{6p}	946	1137 ± 140	1.202
	G^1(4s, 6p)	3563	3555 ± 322	0.998
4s6f	E_{av}	715 526	723 277 ± 115	1.011
	ζ_{6f}	3	3 (FIX)	1.000
	G^3(4s, 6f)	5365	4560 (FIX)	0.850
Configuration interaction integrals				
4s4p–4p 4d	R^2(4s4p, 4d4p)	61 927	46 445 (FIX)	0.750
4p4d–4s4f	R^1(4p4d, 4s4f)	64 971	54 967 (FIX)	0.846
4p4d–4s4f	R^2(4p4d, 4f4s)	43 522	36 846 (FIX)	0.847

Note. (a) F/HF means Fitted/Hartree–Fock. Parameters omitted from this table: direct and exchange integrals, and spin–orbit parameters set for configurations that not have known experimental levels, this values were set to 85%, 85%, and 95% of their HFR values respectively; CI omitted integrals were set to 85% of their HFR values. The standard deviation for energy adjustment was 158 cm^{-1}.

converges smoothly as more correlation is included and it is less sensitive to details of the computational method [24]. This method takes into account relativistic effects by means of a more complete approach than Cowan's package, but the HFR method takes into account correlation effects in a more complete way. In the HFR + CP method, not only are correlation effects considered more deeply, but CP effects are taken into account in the lifetime calculations. These concepts are reflected in table 1 where the calculations for lifetimes of Kr VII considering CP effects (B and C) are in general closer to the experimental values [10, 11] than the calculations A and D. In particular, our calculated lifetime values of the energy levels including CP effects, which we compared with the experimental values of [10, 11], are in better agreement with the values shown as (e y g) in table 1 than the other values reported if we consider the maximum error specified in each case. A technique to remove the effect of cascade repopulation from beam-foil lifetimes measurements (ANDC) were used in such papers. It is possible that if the authors had used these corrections for the levels 4s5p $^1P_1$ 4s5d $^3D_{1,2,3}$ our theoretical values would be closer to the experimental values reported by them.

Our HFR + CP calculated value for the lifetime of the 4s4p $^3P_1$ level is in good agreement with the value reported by Hibbert *et al* [13]. In some cases, where the calculated values are not in agreement with the experimental values as it is for the lifetime of the $4p^2$ $^1D_2$ level and this could be due to the mixing of percentage composition of the levels involved in the calculation [3]. It is noteworthy that in all HFR calculations with and without CP, we considered optimized values of the energy parameters using least squares techniques where we adjusted the theoretical values to the experimental ones.

4. Conclusion

Four different calculations of lifetimes in Kr VII were carried out: A, considering the HFR approach [14] with the modifications very recently suggested by Kramida [12]; B and C, including CP effects HFR + CP [16] and D, using the GRASP code [17]. Three sets of configurations were taken into account in the calculation A, B and C. In the calculation D we considered the same set of configurations as in C. For some energy levels, we compared the lifetimes with the experimental values given in the bibliography [10, 11]. In most cases the HFR + CP calculations are in better agreement with the experimental lifetimes, especially if we consider the maximum error in each case taking into account the ANDC technique, reported in the [10, 11]. The values calculated with the GRASP code (D) are in better accordance with those calculated in the case A, where core excited configurations were included.

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