Lifetime calculations in energy levels of Kr VII

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Keywords: atomic spectroscopy, lifetimes, energy levels

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, 4s5s, 4s6s, 4p4f, 4s4p, 4s5p, 4s6p, 4s6f, 4s5f, 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 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 I isoelectronic sequence [12]. Using configuration interaction wave functions, Hibbert et al [13] presented lifetime calculations of the 4s4p 2P 3/2 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
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 multi-configurational 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 $R^e$ and exchange $G^e$ integrals, effective radial parameter $\alpha$, configuration interaction integrals $R^{fi}$, and spin–orbit parameters $\zeta^{fi}$. 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 $\tau(\gamma f)$ is the inverse of transition probability, then:

$$\tau(\gamma f) = (\sum A(\gamma f, \gamma'f'))^{-1},$$

where $A(\gamma f, \gamma'f')$ 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

$$\int_0^\infty R_{\alpha d}(r)P_{\alpha d}(r)dr \rightarrow \int_0^\infty P_{\alpha d}r \cdot \left[ 1 - \frac{\alpha_d}{(r^2 + r_0^2)^{3/2}} \right]P_{\alpha d}(r)dr - \frac{\alpha_d}{r_0^2} \int_0^{r_0} P_{\alpha d}(r)P_{\alpha d}(r)dr. \tag{2}$$

Here $\alpha_d$ is the electric dipole polarizability of the core, and $r_0$ 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 multi-configurational 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: $4s^5$, $4p^2$, $4s4d$, $4d^2$, $4s5s$, $4s5d$, $4p4f$, $4f^2$, $4p5p$, $4p5f$, $4s6s$, $4s6d$, $3d^24s^24d$ and $4s4p$, $4p4d$, $4s5p$, $4s5f$, $4p5s$, $4p5d$, $4d6p$, $4d6f$, $4d4f$, $3d4s^24p$ 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 $R^{(4s5d,4s6d)}$, $R^{(4s5p,4s6p)}$ and $R^{(4s5f,4s6f)}$ 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 | \( E_{\text{exp}} \) (cm\(^{-1}\)) | \( E_{\text{cal}} \) (cm\(^{-1}\)) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|----------------------------------|----------------------------------|------------------------|--------------------|---------------|---------------------------|
| 4s\(^2\) S\(_0\)       | 0.0                              | 0.0                              | 98                     | A                 | \( \infty \)             | \( \infty \)               |
|               |                                  |                                  |                        | B                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | C                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | D                 | \( \infty \)             |                           |
| 4s4p \(^3\) P\(_0\)   | 117 389.6                        | 117 399                          | 100                    | A                 | \( \infty \)             | \( \infty \)               |
|               |                                  |                                  |                        | B                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | C                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | D                 | \( \infty \)             |                           |
| 4s4p \(^1\) P\(_1\)   | 120 094.8                        | 120 083                          | 99                     | A                 | 38.08                     | 47 \pm 10\(^d\)           |
|               |                                  |                                  |                        | B                 | 45.03                     |                           |
|               |                                  |                                  |                        | C                 | 42.04                     |                           |
|               |                                  |                                  |                        | D                 | 65.75                     |                           |
| 4s4p \(^3\) P\(_2\)   | 126 553.8                        | 126 556                          | 100                    | A                 | \( \infty \)             | \( \infty \)               |
|               |                                  |                                  |                        | B                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | C                 | \( \infty \)             |                           |
|               |                                  |                                  |                        | D                 | \( \infty \)             |                           |
| 4s4p \(^1\) P\(_1\)   | 170 835.0                        | 170 835                          | 97                     | A                 | 0.088                     | 0.101 \pm 0.01\(^e\)      |
|               |                                  |                                  |                        | B                 | 0.104                     |                           |
|               |                                  |                                  |                        | C                 | 0.100                     |                           |
|               |                                  |                                  |                        | D                 | 0.086                     |                           |
| 4p\(^2\) P\(_0\)      | 274 931.7                        | 274 906                          | 96                     | A                 | 0.108                     | 0.158 \pm 0.018\(^f\)     |
|               |                                  |                                  |                        | B                 | 0.119                     |                           |
|               |                                  |                                  |                        | C                 | 0.127                     |                           |
|               |                                  |                                  |                        | D                 | 0.107                     |                           |
| 4p\(^2\) P\(_1\)      | 279 414.5                        | 279 449                          | 100                    | A                 | 0.102                     | 0.156 \pm 0.025\(^f\)     |
|               |                                  |                                  |                        | B                 | 0.112                     |                           |
|               |                                  |                                  |                        | C                 | 0.121                     |                           |
|               |                                  |                                  |                        | D                 | 0.102                     |                           |
| 4p\(^2\) P\(_2\)      | 288 190.2                        | 288 172                          | 67 4p\(^3\) P + 28 4p\(^2\) D + 5 4s4d\(^1\) D | A                 | 0.130                     | 0.173 \pm 0.015\(^f\)     |
|               |                                  |                                  |                        | B                 | 0.144                     |                           |
|               |                                  |                                  |                        | C                 | 0.155                     |                           |
|               |                                  |                                  |                        | D                 | 0.343                     |                           |
| 4p\(^1\) D\(_2\)      | 279 714.8                        | 279 723                          | 59 4p\(^2\) D + 32 4p\(^2\) P + 8 4s4d\(^1\) D | A                 | 0.240                     | 0.081 \pm 0.020\(^f\)     |
|               |                                  |                                  |                        | B                 | 0.267                     |                           |
|               |                                  |                                  |                        | C                 | 0.287                     |                           |
| Designation | $E_{\text{exp}}$ (cm$^{-1}$) | $E_{\text{cal}}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|-----------------|-----------------|-----------------|-----------------|--------------|---------------------|
| 4p$^2$1S$_0$ | 321 794.0       | 321 795         | 94              | D               | 0.118        |                     |
|             |                 |                 |                 | A               | 0.096        |                     |
|             |                 |                 |                 | B               | 0.104        |                     |
|             |                 |                 |                 | C               | 0.113        |                     |
|             |                 |                 |                 | D               | 0.096        |                     |
| 4s4d $^3$D$_1$ | 349 973.1       | 350 067         | 100             | A               | 0.043        |                     |
|             |                 |                 |                 | B               | 0.045        |                     |
|             |                 |                 |                 | C               | 0.049        |                     |
|             |                 |                 |                 | D               | 0.044        |                     |
| 4s4d $^3$D$_2$ | 350 416.8       | 350 435         | 100             | A               | 0.045        |                     |
|             |                 |                 |                 | B               | 0.047        |                     |
|             |                 |                 |                 | C               | 0.050        |                     |
|             |                 |                 |                 | D               | 0.045        |                     |
| 4s4d $^3$D$_3$ | 351 116.2       | 351 004         | 100             | A               | 0.048        |                     |
|             |                 |                 |                 | B               | 0.049        |                     |
|             |                 |                 |                 | C               | 0.053        |                     |
|             |                 |                 |                 | D               | 0.047        |                     |
| 4s4d $^1$D$_2$ | 379 488.3       | 379 489         | $85\, 4s4d\, ^1D + 13\, 4p^2\, ^1D$ | A               | 0.033        | 0.046 ± 0.008$^d$  |
|             |                 |                 |                 | B               | 0.034        |                     |
|             |                 |                 |                 | C               | 0.037        |                     |
|             |                 |                 |                 | D               | 0.033        |                     |
| 4s5s $^3$S$_1$ | 438 644         | 438 636         | 99              | A               | 0.037        |                     |
|             |                 |                 |                 | B               | 0.030        |                     |
|             |                 |                 |                 | C               | 0.033        |                     |
|             |                 |                 |                 | D               | 0.039        |                     |
| 4s5s $^1$S$_0$ | 447 769         | 447 777         | 99              | A               | 0.050        |                     |
|             |                 |                 |                 | B               | 0.042        |                     |
|             |                 |                 |                 | C               | 0.047        |                     |
|             |                 |                 |                 | D               | 0.056        |                     |
| 4p4d $^3$F$_2$ | 475 890         | 475 922         | $88\, 4p4d\, ^3F + 7\, 4p4d\, ^1D + 5\, 4s4f\, ^1F$ | A               | 0.527        |                     |
|             |                 |                 |                 | B               | 0.643        |                     |
|             |                 |                 |                 | C               | 0.644        |                     |
|             |                 |                 |                 | D               | 0.725        |                     |
| 4p4d $^3$F$_3$ | 479 655         | 479 663         | $92\, 4p4d\, ^3F + 6\, 4s4f\, ^1F$ | A               | 0.720        |                     |
|             |                 |                 |                 | B               | 0.898        |                     |
|             |                 |                 |                 | C               | 0.902        |                     |
| Designation | $E_{\text{exp}}$ (cm$^{-1}$) | $E_{\text{ad}}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|-----------------|-----------------|----------------------|------------------|--------------|---------------------------|
| 4p4d $^3$F$_4$ | 484 543 | 484 542 | $92 \, 4p4d \, ^3F + 8 \, 4s4f \, ^3F$ | D | 1.005 | |
|             |           |           |                     | A | 1.117 | |
|             |           |           |                     | B | 1.500 | |
|             |           |           |                     | C | 1.522 | |
|             |           |           |                     | D | 1.510 | |
| 4p4d $^1$F$_3$ | 505 076 | 505 016 | $36 \, 4p4d \, ^1F + 34 \, 4s4f \, ^1F + 29 \, 4p4d \, ^3D$ | A | 0.033 | |
|             |           |           |                     | B | 0.039 | |
|             |           |           |                     | C | 0.039 | |
|             |           |           |                     | D | 0.029 | |
| 4p4d $^3$D$_2$ | 501 542 | 501 553 | $65 \, 4p4d \, ^1D + 28 \, 4p4d \, ^3P$ | A | 0.030 | |
|             |           |           |                     | B | 0.036 | |
|             |           |           |                     | C | 0.034 | |
|             |           |           |                     | D | 0.032 | |
| 4p4d $^3$D$_3$ | 507 934 | 507 873 | $62 \, 4p4d \, ^1D + 36 \, 4p4d \, ^3P$ | A | 0.030 | |
|             |           |           |                     | B | 0.034 | |
|             |           |           |                     | C | 0.034 | |
|             |           |           |                     | D | 0.037 | |
| 4p4d $^3$D$_4$ | 508 473 | 508 595 | $70 \, 4p4d \, ^1D + 16 \, 4s4f \, ^1F + 13 \, 4p4d \, ^3F$ | A | 0.032 | |
|             |           |           |                     | B | 0.036 | |
|             |           |           |                     | C | 0.036 | |
|             |           |           |                     | D | 0.041 | |
| 4p4d $^1$D$_2$ | 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 $^3$P$_0$ | 506 933 | 506 938 | 97 | A | 0.037 | |
|             |           |           |                     | B | 0.042 | |
|             |           |           |                     | C | 0.042 | |
|             |           |           |                     | D | 0.039 | |
| 4p4d $^3$P$_1$ | 507 446 | 507 448 | $66 \, 4p4d \, ^3P + 32 \, 4p4d \, ^3D$ | A | 0.033 | |
|             |           |           |                     | B | 0.037 | |
|             |           |           |                     | C | 0.037 | |
|             |           |           |                     | D | 0.034 | |
| 4p4d $^3$P$_2$ | 501 769 | 501 763 | $52 \, 4p4d \, ^3P + 35 \, 4p4d \, ^3D + 7 \, 4s5p \, ^3P$ | A | 0.035 | |
|             |           |           |                     | B | 0.039 | |
|             |           |           |                     | C | 0.039 | |

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| Designation | $E_{exp}$ (cm$^{-1}$) | $E_{	ext{ad}}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|----------------------|-----------------------------|------------------------|----------------------|--------------|---------------------------|
| 4p4d $1^1P_1$ | 535 462 | 535 465 | 94 | D | 0.031 | 0.037 |
| | | | | A | 0.043 | 0.043 |
| | | | | B | 0.045 | 0.043 |
| | | | | C | 0.043 | 0.043 |
| | | | | D | 0.038 | 0.038 |
| 4s5p $1^3P_1$ | 492 776 | 492 735 | 97 | A | 0.235 ± 0.040 | 0.330 ± 0.040 |
| | | | | B | 0.224 | 0.224 |
| | | | | C | 0.225 | 0.225 |
| | | | | D | 0.250 | 0.250 |
| 4s5p $1^3P_2$ | 493 219 | 493 242 | 86 4s5p $^3P + 10 4s5p ^1P$ | A | 0.209 | 0.497 ± 0.040 |
| | | | | B | 0.189 | 0.305 ± 0.040 |
| | | | | C | 0.189 | 0.305 ± 0.040 |
| | | | | D | 0.218 | 0.305 ± 0.040 |
| 4s5p $1^3P_3$ | 495 578.4 | 495 580 | 90 4s5p $^3P + 7 4p4d ^3P$ | A | 0.223 | 0.510 ± 0.030 |
| | | | | B | 0.217 | 0.30 ± 0.08 |
| | | | | C | 0.219 | 0.30 ± 0.08 |
| | | | | D | 0.234 | 0.30 ± 0.08 |
| 4s5p $1^3P_4$ | 497 395 | 497 392 | 84 4s5p $^1P + 9 4s5p ^3P$ | A | 0.097 | 0.289 ± 0.040 |
| | | | | B | 0.078 | 0.289 ± 0.040 |
| | | | | C | 0.078 | 0.289 ± 0.040 |
| | | | | D | 0.096 | 0.289 ± 0.040 |
| 4s4f $1^3F_2$ | 530 349 | 530 285 | 94 4s4f $^3F + 6 4p4d ^3F$ | A | 0.045 | 0.045 |
| | | | | B | 0.047 | 0.047 |
| | | | | C | 0.047 | 0.047 |
| | | | | D | 0.045 | 0.045 |
| 4s4f $1^3F_3$ | 530 491 | 530 504 | 93 4s4f $^3F + 7 4p4d ^3F$ | A | 0.044 | 0.044 |
| | | | | B | 0.047 | 0.047 |
| | | | | C | 0.047 | 0.047 |
| | | | | D | 0.045 | 0.045 |
| 4s4f $1^3F_4$ | 530 772 | 530 822 | 92 4s4f $^3F + 8 4p4d ^3F$ | A | 0.044 | 0.044 |
| | | | | B | 0.047 | 0.047 |
| | | | | C | 0.047 | 0.047 |
| | | | | D | 0.044 | 0.044 |
| 4s4f $1^1F_3$ | 560 671 | 560 664 | 49 4s4f $^1F + 48 4p4d ^1F$ | A | 0.024 | 0.024 |
| | | | | B | 0.026 | 0.026 |
| | | | | C | 0.026 | 0.026 |
| Designation | $E_{\text{ex}}$ (cm$^{-1}$) | $E_{\text{id}}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|----------------|----------------|----------------------|----------------|--------------|---------------------------|
| 4s5d $^3\text{D}_1$ | 578 470 | 578 518 | 98 | D | 0.024 | |
| | | | | A | 0.237 | $0.426 \pm 0.030^f$ |
| | | | | B | 0.241 | |
| | | | | C | 0.250 | |
| | | | | D | 0.253 | |
| 4s5d $^3\text{D}_2$ | 578 722 | 578 728 | 98 | A | 0.241 | $0.437 \pm 0.030^f$ |
| | | | | B | 0.245 | |
| | | | | C | 0.254 | |
| | | | | D | 0.255 | |
| 4s5d $^3\text{D}_3$ | 579 109 | 579 056 | 99 | A | 0.249 | $0.491 \pm 0.030^f$ |
| | | | | B | 0.255 | |
| | | | | C | 0.262 | |
| | | | | D | 0.263 | |
| 4s5d $^1\text{D}_2$ | 581 038 | 581 038 | 96 | A | 0.210 | |
| | | | | B | 0.227 | |
| | | | | C | 0.236 | |
| | | | | D | 0.216 | |
| 4p5s $^3\text{P}_0$ | 585 764 | | 99 | A | 0.051 | |
| | | | | B | 0.049 | |
| | | | | C | 0.049 | |
| | | | | D | 0.050 | |
| 4p5s $^3\text{P}_1$ | 587 029 | 587 029 | $84 \text{4p5s}\,^3\text{P} + 14 \text{4p5s}\,^1\text{P}$ | A | 0.045 | |
| | | | | B | 0.042 | |
| | | | | C | 0.043 | |
| | | | | D | 0.046 | |
| 4p5s $^1\text{P}_2$ | 594 617 | 594 617 | 99 | A | 0.047 | |
| | | | | B | 0.045 | |
| | | | | C | 0.045 | |
| | | | | D | 0.048 | |
| 4p5s $^1\text{P}_1$ | 598 281 | 598 281 | $79 \text{4p5s}\,^1\text{P} + 15 \text{4p5s}\,^3\text{P}$ | A | 0.029 | |
| | | | | B | 0.027 | |
| | | | | C | 0.027 | |
| | | | | D | 0.028 | |
| 4s6s $^3\text{S}_1$ | 616 314 | 616 314 | 99 | A | 0.055 | |
| | | | | B | 0.046 | |
| | | | | C | 0.047 | |
Table 1. (Continued.)

| Designation | $E_{exp}$ (cm$^{-1}$) | $E_{ad}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|----------------------|----------------------|------------------------|---------------------|--------------|---------------------------|
| 4s6s$^1$S$_0$ | 618 693 | 618 693 | 98 | D | 0.052 |
|              |                   |                      |                        | A                    | 0.064 |
|              |                   |                      |                        | B                    | 0.056 |
|              |                   |                      |                        | C                    | 0.061 |
|              |                   |                      |                        | D                    | 0.072 |
| 4s5f$^3$F$_2$ | 656 725 | 656 803 | 99 | A | 0.203 |
|              |                   |                      |                        | B                    | 0.212 |
|              |                   |                      |                        | C                    | 0.213 |
|              |                   |                      |                        | D                    | 0.220 |
| 4s5f$^3$F$_3$ | 656 868 | 656 845 | 99 | A | 0.203 |
|              |                   |                      |                        | B                    | 0.212 |
|              |                   |                      |                        | C                    | 0.213 |
|              |                   |                      |                        | D                    | 0.222 |
| 4s5f$^3$F$_4$ | 656 956 | 656 901 | 99 | A | 0.203 |
|              |                   |                      |                        | B                    | 0.213 |
|              |                   |                      |                        | C                    | 0.214 |
|              |                   |                      |                        | D                    | 0.223 |
| 4s5f$^1$F$_3$ | 659 927 | 659 919 | 96 | A | 0.177 |
|              |                   |                      |                        | B                    | 0.187 |
|              |                   |                      |                        | C                    | 0.188 |
|              |                   |                      |                        | D                    | 0.170 |
| 4p4f$^3$G$_5$ | 671 908 | 671 921 | $47 4p4f^3G + 31 4p4f^1F + 20 4p4f^2F$ | A | 0.049 |
|              |                   |                      |                        | B                    | 0.048 |
|              |                   |                      |                        | C                    | 0.054 |
|              |                   |                      |                        | D                    | 0.049 |
| 4p4f$^3$G$_6$ | 673 646 | 674 921 | $63 4p4f^1G + 24 4p4f^3G + 9 4d^2F$ | A | 0.070 |
|              |                   |                      |                        | B                    | 0.067 |
|              |                   |                      |                        | C                    | 0.078 |
|              |                   |                      |                        | D                    | 0.037 |
| 4p4f$^3$G$_7$ | 671 786 | 671 786 | $100$ | A | 0.050 |
|              |                   |                      |                        | B                    | 0.047 |
|              |                   |                      |                        | C                    | 0.053 |
|              |                   |                      |                        | D                    | 0.050 |
| 4p4f$^3$G$_8$ | 671 378 | 671 351 | $46 4p4f^3F + 30 4p4f^1G + 11 4d^2F$ | A | 0.094 |
|              |                   |                      |                        | B                    | 0.093 |
|              |                   |                      |                        | C                    | 0.106 |
| Designation | \(E_{\text{exp}} \text{ (cm}^{-1}\text{)}\) | \(E_{\text{cal}} \text{ (cm}^{-1}\text{)}\) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|-----------------|-----------------|---------------------|-------------------|---------------|-----------------------------|
| 4p4f \^{3}\F_{2} | 664 923 | 665 007 | 86 4p4f \^{1}\F + 7 \text{4d}^{2}\F | D | 0.118 | |
| 4p4f \^{3}\F_{3} | 664 997 | 664 897 | 49 4p4f \^{3}\F + 38 4p4f \^{1}\F + 9 4p4f \^{3}\D | A | 0.023 | B | 0.042 | C | 0.047 | D | 0.048 |
| 4p4f \^{1}\F_{4} | 663 983 | 664 015 | 43 4p4f \^{1}\F + 28 4p4f \^{3}\G + 21 4p4f \^{1}\G | A | 0.023 | B | 0.042 | C | 0.047 | D | 0.048 |
| 4p4f \^{3}\D_{1} | 684 070 | 684 002 | 99 | A | 0.043 | B | 0.042 | C | 0.047 | D | 0.048 |
| 4p4f \^{3}\D_{2} | 681 681 | 681 336 | 65 4p4f \^{3}\D + 23 4p4f \^{1}\D + 6 \text{4d}^{2}\F | A | 0.046 | B | 0.045 | C | 0.050 | D | 0.049 |
| 4p4f \^{3}\D_{3} | 680 086 | 680 361 | 89 4p4f \^{1}\D + 5 4p4f \^{3}\F + 4 4p4f \^{3}\F | A | 0.046 | B | 0.045 | C | 0.050 | D | 0.049 |
| 4p4f \^{1}\D_{2} | 684 941 | 685 081 | 54 4p4f \^{1}\D + 31 4p4f \^{3}\D + 13 \text{4d}^{2}\D | A | 0.046 | B | 0.046 | C | 0.050 | D | 0.055 |
| 4s6p \^{3}\P_{0} | 640 160 | 640 334 | 100 | A | 0.258 | B | 0.241 | C | 0.242 |
Table 1. (Continued.)

| Designation | $E_{\text{exp}}$ (cm$^{-1}$) | $E_{\text{cal}}$ (cm$^{-1}$) | Percentage composition | Type of calculation | Lifetime (ns) | Experimental lifetime (ns) |
|-------------|-------------------------------|-------------------------------|------------------------|---------------------|---------------|---------------------------|
| $4s^6 3P_1$ | 640 761                       | 640 780                       | 97                     | D                   | 0.240         |                           |
|             |                               |                               |                        | A                   | 0.251         |                           |
|             |                               |                               |                        | B                   | 0.231         |                           |
|             |                               |                               |                        | C                   | 0.232         |                           |
|             |                               |                               |                        | D                   | 0.233         |                           |
| $4s^6 3P_2$ | 642 010                       | 642 050                       | 100                    | A                   | 0.248         |                           |
|             |                               |                               |                        | B                   | 0.232         |                           |
|             |                               |                               |                        | C                   | 0.233         |                           |
|             |                               |                               |                        | D                   | 0.238         |                           |
| $4s^6 1P_1$ | 645 430                       | 645 423                       | 94                     | A                   | 0.140         |                           |
|             |                               |                               |                        | B                   | 0.104         |                           |
|             |                               |                               |                        | C                   | 0.105         |                           |
|             |                               |                               |                        | D                   | 0.130         |                           |
| $4s^6 3D_1$ | 694 858                       | 694 857                       | 99                     | A                   | 0.239         |                           |
|             |                               |                               |                        | B                   | 0.236         |                           |
|             |                               |                               |                        | C                   | 0.251         |                           |
|             |                               |                               |                        | D                   | 0.195         |                           |
| $4s^6 1D_2$ | 695 056                       | 694 957                       | 99                     | A                   | 0.242         |                           |
|             |                               |                               |                        | B                   | 0.240         |                           |
|             |                               |                               |                        | C                   | 0.255         |                           |
|             |                               |                               |                        | D                   | 0.217         |                           |
| $4s^6 3D_3$ | 695 015                       | 695 115                       | 99                     | A                   | 0.248         |                           |
|             |                               |                               |                        | B                   | 0.247         |                           |
|             |                               |                               |                        | C                   | 0.263         |                           |
|             |                               |                               |                        | D                   | 0.299         |                           |
| $4s^6 1D_2$ | 697 330                       | 697 330                       | 94                     | A                   | 0.205         |                           |
|             |                               |                               |                        | B                   | 0.192         |                           |
|             |                               |                               |                        | C                   | 0.207         |                           |
|             |                               |                               |                        | D                   | 0.128         |                           |
| $4s^6 3F_2$ | 724 718                       | 724 629                       | 78 4s6f$^3$F$^+$ 17 4p5d$^3$F$^+$ | A | 0.273 |                           |
|             |                               |                               |                        | B                   | 0.303         |                           |
|             |                               |                               |                        | C                   | 0.305         |                           |
|             |                               |                               |                        | D                   | 0.160         |                           |
| $4s^6 3F_3$ | 724 826                       | 725 127                       | 69 4s6f$^3$F$^+$ 24 4p5d$^3$F$^+$ 4p5d$^3$D$^+$ | 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) |
|-------------|----------------|----------------|-----------------|------------------|--------------|---------------------------|
| 4s6f$^1$F$_4$ | 725 989 | 726 069 | 59 4s6f$^3$F + 40 4p5d$^3$F | D | 0.432 |  |
| | | | | A | 0.189 |  |
| | | | | B | 0.210 |  |
| | | | | C | 0.205 |  |
| | | | | D | 0.454 |  |
| 4s6f$^1$F$_3$ | 719 130 | 718 791 | 42 4s6f$^1$F + 22 4p5d$^1$F + 15 4p5d$^3$F | 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].
$^d$ Experimental lifetimes reported by Pinnington [10].
$^e$ 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.
The dipole polarizability of the ionic core, \( \alpha_{\text{d}} \), 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. \( \alpha_{\text{d}} = 0.209 \alpha_0 \), 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 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, \( \alpha_{\text{d}} \), 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. \( \alpha_{\text{d}} = 0.209 \alpha_0 \), 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 (\( E_{\text{av}}, F^2, G^2, G^4 \)) were held 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–4f4p and 5s\(^2 \)–5p\(^4 \) that were held fixed at 75% of their HF values. For the odd parity, all parameters (\( E_{\text{av}}, F^2, G^2, G^4 \)) were left free for the known configurations except for the \( G^2(4s,6f) \) 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

| Configuration | Parameter | HF value | Fitted value | \( F/\text{HF} \) |
|---------------|-----------|----------|--------------|----------------|
| \( 4s^2 \)    | \( E_{\text{av}} \) | 0.0      | 7319 ± 158   | 1.034         |
| \( 4p^2 \)    | \( E_{\text{av}} \) | 281 386  | 290 937 ± 90 | 1.034         |
| \( 4s4d \)    | \( E_{\text{av}} \) | 403      | 383 (FIX)    | 0.950         |
| \( 4s5s \)    | \( G^2(4s,4d) \) | 53 495   | 47 443 ± 523 | 0.886         |
| \( 4s5d \)    | \( G^2(4s,5s) \) | 6340     | 5311 ± 111   | 0.838         |
| \( 4p4f \)    | \( G^2(4s,5d) \) | 11 272   | 9785 ± 469   | 0.868         |

| Configuration interaction integrals |
|------------------------------------|
| \( 4s4d–4f4p \) | \( R^2(4s4d,4f4p) \) |
| \( 5s^2–5p^4 \) | \( R^2(5s5s,5p5p) \) |

Table 2. Energy parameters (cm\(^{-1} \)) for the studied even parity configurations in the calculation C of Kr\(^{7+} \).
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 as it is for the lifetime of the 4p 2 1 D 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 values.

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 | E/HF(a) |
|---------------|-----------|----------|--------------|---------|
| 4s4p          | E\(_{\text{av}}\) | 127 325  | 137 895 ± 87 | 1.083   |
|               | \(\xi_p\)     | 5500     | 6130 ± 144   | 1.114   |
|               | \(G^{(4s, 4p)}\) | 93 862  | 79 316 ± 299 | 0.845   |
| 4p4d         | E\(_{\text{av}}\) | 490 335  | 502 378 ± 55 | 1.024   |
|               | \(\xi_p\)     | 5601     | 6258 ± 120   | 1.117   |
|               | \(\xi_d\)     | 413      | 392 (FIX)    | 0.950   |
|               | \(F^{(4p, 4d)}\) | 60 639  | 54 845 ± 513 | 0.904   |
|               | \(G^{(4p, 4d)}\) | 74 858  | 65 164 ± 273 | 0.870   |
|               | \(G^{(4p, 4d)}\) | 46 888  | 41 677 ± 455 | 0.899   |
| 4s5p         | E\(_{\text{av}}\) | 487 599  | 497 486 ± 94 | 1.020   |
|               | \(\xi_p\)     | 1950     | 2055 ± 141   | 1.054   |
|               | \(G^{(4s, 5p)}\) | 9827    | 7661 ± 389   | 0.779   |
| 4s4f         | E\(_{\text{av}}\) | 518 166  | 528 984 ± 108| 1.021   |
|               | \(\xi_f\)     | 8        | 8 (FIX)      | 1.000   |
|               | \(G^{(4s, 4f)}\) | 26 286  | 22 919 ± 1208| 0.872   |
| 4s5f         | E\(_{\text{av}}\) | 646 259  | 658 081 ± 81 | 1.018   |
|               | \(\xi_f\)     | 5        | 5 (FIX)      | 1.000   |
|               | \(G^{(4s, 5f)}\) | 10 763  | 10 392 ± 663 | 0.965   |
| 4p5s         | E\(_{\text{av}}\) | 581 531  | 592 396 ± 95 | 1.019   |
|               | \(\xi_p\)     | 5803     | 5938 ± 149   | 1.023   |
|               | \(G^{(4p, 5s)}\) | 9110    | 6550 ± 407   | 0.719   |
| 4s6p         | E\(_{\text{av}}\) | 634 019  | 641 988 ± 87 | 1.012   |
|               | \(\xi_p\)     | 946      | 1137 ± 140   | 1.202   |
|               | \(G^{(4s, 6p)}\) | 3563    | 3555 ± 322   | 0.998   |
| 4s6f         | E\(_{\text{av}}\) | 715 526  | 723 277 ± 115| 1.011   |
|               | \(\xi_f\)     | 3        | 3 (FIX)      | 1.000   |
|               | \(G^{(4s, 6f)}\) | 5365    | 4560 (FIX)   | 0.850   |

Note. (a) E/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\(^{-1}\).
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 [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.

Acknowledgments

E Grumel and L Cap, who helped us in the Cowan code modification suggested by Kramida [15], are gratefully acknowledged. The Comisión de Investigaciones Científicas de la Provincia de Buenos Aires, Argentina, where MR and JRA are researchers, is gratefully acknowledged. The research was also supported by the Universidade Federal de Roraima (UFRR), Boa Vista, Brazil where EEF is researcher.

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