

MCDHF and RCI calculations of energy levels, lifetimes and transition rates for $3l3l'$, $3l4l'$, and $3s5l$ states in Ca IX – As XXII and Kr XXV[★]

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ABSTRACT

Multiconfiguration Dirac-Hartree-Fock (MCDHF) calculations and relativistic configuration interaction (RCI) calculations were performed for states of the $3l3l'$, $3l4l'$ and $3s5l$ configurations in the Mg-like ions Ca IX – As XXII and Kr XXV. Valence and core-valence electron correlation effects are accounted for through large configuration state function expansions. Calculated excitation energies are in very good agreement with observations for the lowest levels. For higher lying levels observations are often missing and present energies aid line identification in spectra. Lifetimes and transition data are given for all ions. There is an excellent agreement for both lifetimes and transition data with recent multiconfiguration Hartree-Fock Breit Pauli calculations.

Key words. atomic data – methods: numerical – line: identification

1. Introduction

Mg-like ions are of considerable interest for diagnostic purposes in astrophysical plasmas and in fusion plasmas. The background and diagnostic details are given in Aggarwal et al. (2007) as well as in a series of comprehensive papers by Landi and Bhatia (Landi & Bhatia 2014; Bhatia & Landi 2011; Landi 2011).

During the past years a large number of calculations have been performed for Mg-like ions. In addition to the calculations above, see for example, Safronova et al. (2000), Froese Fischer et al. (2006), Massacrier & Artru (2012), Hu et al. (2014), Si et al. (2015), Santana & Träbert (2015). The most recent R-matrix calculations for the Mg-like ions include both collisional and radiative data (Fernandez-Mencheró et al. 2014). Some of the calculations above provided data only for levels in the $n = 3$ complex but, as pointed out by Landi (2011), the real need is for data involving configurations with $n \geq 4$.

In addition to energies and transition data involving configurations with $n \geq 4$, there is also a need for transition energies that are accurate enough to aid line identifications. To meet these needs, systematic large scale relativistic multiconfiguration calculations were performed for states belonging to the $3l3l'$, $3l4l'$ and $3s5l$ configurations in the ions Ca IX – As XXII and Kr XXV. The present calculations provide a consistent and accurate data set for line identification and modeling purposes. The data set can also be used as a benchmark for other calculations.

[★] Tables for energy levels, lifetimes, and transition data and full Tables 2, 4, and 6 are available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/597/A76>

2. Relativistic multiconfiguration calculations

The calculations were performed using the four-component fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) method relying on multireference single and double (MRSD) substitutions for generating wave function expansions. The method is described in detail in (Grant 2007) and in a recent review of multiconfiguration methods (Froese Fischer et al. 2016).

2.1. Multiconfiguration Dirac-Hartree-Fock

An atomic state is described by a wave function Ψ , that is a solution to the wave equation based on the Dirac-Coulomb Hamiltonian. In the MCDHF method, the wave function $\Psi(\gamma P J M)$ for a state labeled $\gamma P J M$ with γ being the orbital occupancy and angular coupling scheme, P the parity, and J and M the total angular quantum numbers, is expanded in configuration state functions (CSFs)

$$\Psi(\gamma P J M) = \sum_{j=1}^{N_{\text{CSF}}} c_j \Phi(\gamma_j P J M). \quad (1)$$

The CSFs are antisymmetrized and symmetry-adapted many electron functions built from products of one-electron Dirac orbitals (Grant 2007; Froese Fischer et al. 2016).

The wave functions were determined in the extended optimal level (EOL) scheme and the radial parts of the Dirac orbitals and the expansion coefficients of the studied states were obtained iteratively in a layer by layer approach, as specified in Sect. 2.3, from a set of equations that results from applying the variational

Table 1. Calculated excitation energies including low-frequency Breit and QED effects in cm^{-1} for Fe XV as a function of the increasing size of the CSF expansion.

Level	MR	$n = 6$	$n = 7$	$n = 8$	E_{NIST}	ΔE
$3s^2 \ ^1S_0$	0	0	0	0	0	0
$3s3p \ ^3P_0^\circ$	234 093	232 715	233 776	233 828	233 842	-14
$3s3p \ ^3P_1^\circ$	239 939	238 571	239 617	239 668	239 660	8
$3s3p \ ^3P_2^\circ$	254 097	252 628	253 774	253 829	253 820	9
$3s3p \ ^1P_1^\circ$	353 073	356 546	352 320	352 169	351 911	258
$3p^2 \ ^3P_0$	554 967	556 652	554 630	554 643	554 524	119
$3p^2 \ ^1D_2$	560 057	559 954	559 805	559 834	559 600	234
$3p^2 \ ^3P_1$	564 964	566 472	564 636	564 663	564 602	61
$3p^2 \ ^3P_2$	582 186	583 268	581 903	581 933	581 803	130
$3p^2 \ ^1S_0$	661 647	666 086	660 598	660 269	659 627	642
$3s3d \ ^3D_1$	678 934	681 357	678 918	678 954	678 772	182
$3s3d \ ^3D_2$	679 960	682 353	679 948	679 986	679 785	201
$3s3d \ ^3D_3$	681 569	683 911	681 562	681 603	681 416	187
$3s3d \ ^1D_2$	764 433	771 831	763 242	762 729	762 093	636
$3p3d \ ^3F_2^\circ$	928 976	929 572	928 467	928 565	928 241	324
$3p3d \ ^3F_3^\circ$	938 881	939 360	938 373	938 469	938 126	343
$3p3d \ ^1D_2^\circ$	949 099	950 319	948 656	948 768	948 513	255
$3p3d \ ^3F_4^\circ$	950 379	950 744	949 888	949 990	949 658	332
$3p3d \ ^3D_1^\circ$	983 762	987 307	983 044	983 077	982 868	209
$3p3d \ ^3P_2^\circ$	984 401	987 628	983 723	983 765	983 514	251
$3p3d \ ^3D_3^\circ$	995 717	999 181	995 041	995 088	994 852	236
$3p3d \ ^3P_0^\circ$	996 918	1 000 006	996 184	996 218	995 889	329
$3p3d \ ^3P_1^\circ$	997 231	1 000 416	996 509	996 547	996 243	304
$3p3d \ ^3D_2^\circ$	997 548	1 000 823	996 849	996 892	996 623	269
$3p3d \ ^1F_3^\circ$	1 065 486	1 072 573	1 063 598	1 063 163	1 062 515	648
$3p3d \ ^1P_1^\circ$	1 078 724	1 086 604	1 076 426	1 075 795	1 074 887	908
$3d^2 \ ^3F_2$	1 370 858	1 374 588	1 370 811	1 370 858	1 370 331	527
$3d^2 \ ^3F_3$	1 372 524	1 376 182	1 372 476	1 372 527	1 372 035	492
$3d^2 \ ^3F_4$	1 374 560	1 378 157	1 374 525	1 374 580	1 374 056	524
$3d^2 \ ^1D_2$	1 404 365	1 409 904	1 403 685	1 403 474	1 402 592	882
$3d^2 \ ^3P_0$	1 406 561	1 411 610	1 406 345	1 406 328		
$3d^2 \ ^3P_1$	1 407 198	1 412 173	1 406 940	1 406 926		
$3d^2 \ ^1G_4$	1 409 313	1 415 257	1 408 270	1 407 974	1 407 058	916
$3d^2 \ ^3P_2$	1 408 806	1 413 825	1 408 503	1 408 467	1 407 773	694
$3d^2 \ ^1S_0$	1 491 776	1 500 820	1 489 804	1 488 993	1 487 054	1939

Notes. Expansions are obtained from CSFs that can be generated from SD excitations, from an MR, to an active set labeled by the highest n value of the of orbitals in the set. Observed energies are from the NIST Atomic Spectra Database (ver. 5.3; [Kramida et al. 2015](#)). ΔE is the difference between the calculated energies for $n = 8$ and the observed energies.

principle on a weighted energy functional of the studied states together with terms for preserving the orthonormality of the orbitals ([Dyall et al. 1989](#)). The transverse photon interaction in the low-frequency limit, or the Breit interaction ([McKenzie et al. 1980](#)), the mass polarization terms and the leading quantum electrodynamic (QED) effects (vacuum polarization and self-energy) were included in subsequent configuration interaction (RCI) calculations. In the RCI calculations the Dirac orbitals from the previous step were fixed, and only the expansion coefficients of the CSFs were determined by diagonalizing the Hamiltonian matrix. All calculations were performed with an updated parallel version of the GRASP2K code ([Jönsson et al. 2013b](#)).

2.2. Transition parameters

Transition parameters, such as transition rates or weighted oscillator strengths, between two states $\gamma'P'J'$ and γPJ , were

expressed in terms of matrix elements of the transition operator ([Grant 1974](#)). In cases where the wave functions of the two states $\gamma'P'J'$ and γPJ were separately determined there are two orbital sets; one orbital set for $\gamma'P'J'$ and another orbital set for γPJ . Whereas the orbitals are orthonormal within each orbital set, orbitals for $\gamma'P'J'$ are not orthonormal to orbitals for γPJ . This complicates the evaluation of the matrix elements. To deal with this, the wave functions of the two states were transformed so that the orbital sets became biorthonormal ([Olsen et al. 1995](#); [Jönsson & Froese Fischer 1998](#)), after which the calculation of the matrix elements was done using standard Racah algebra methods.

For electric multipole transitions, there are two forms of the transition operator: the length form and the velocity form ([Grant 1974](#)). Although the terms length and velocity form are applicable only to nonrelativistic calculations, in this paper we use them instead of the equivalent Babushkin and Coulomb gauges that

are used in fully relativistic calculations such as ours. The length form is usually preferred, although the velocity form seems to be more stable for transitions including highly excited Rydberg states. The agreement between transition rates A_l and A_v computed in length and velocity forms can be used as an independent check on the accuracy of the wave functions that can be applied even when no values from observation are available (Froese Fischer 2009; Ekman et al. 2014). In this work the quantities

$$dA = \frac{|A_l - A_v|}{\max(A_l, A_v)} \quad \text{and} \quad dT = \frac{|\tau_l - \tau_v|}{\max(\tau_l, \tau_v)}, \quad (2)$$

were used as accuracy indicators for the transition rates and the lifetimes, respectively. The uncertainty indicators cannot be applied to a particular transition or level, but should instead be used in a statistical manner. The average root-mean-square (rms) value of the uncertainty indicator for a group of transitions that are similar in some sense can be used as an estimate for the uncertainty of transitions in this group. This is further discussed in Sect. 3.3.

2.3. Calculations

Calculations were performed for states belonging to the $3s^2$, $3p^2$, $3s3d$, $3d^2$, $3s4s$, $3s4d$, $3p4p$, $3p4f$, $3d4s$, $3d4d$, $3s5s$, $3s5d$, $3s5g$ even configurations and the $3s3p$, $3p3d$, $3s4p$, $3p4s$, $3s4f$, $3p4d$, $3d4p$, $3d4f$, $3s5p$, $3s5f$ odd configuration. These configurations define the multireference (MR) for the even and odd parities, respectively. As a starting point an MCDHF calculation for all even and odd reference states was done in the EOL scheme. The initial calculation was followed by separate calculations in the EOL scheme for the even and odd parity states. The calculations for the even states were based on CSF expansions obtained by allowing single (S) and double (D) substitutions of orbitals in the even MR configurations to an increasing active set of orbitals. In a similar way the calculations for the odd states were based on CSF expansions obtained by allowing single (S) and double (D) substitutions of orbitals in the odd MR configurations to an increasing active set of orbitals. To prevent the CSF expansions to grow unmanageably large, at most single substitutions were allowed from the $2s$ and $2p$ subshells. The $1s$ shell was always closed. The CSF expansions account for valence and core-valence electron correlation. Remaining correlation effects, mainly core-core correlation, are comparatively unimportant for both the excitation energies and the transition probabilities for such highly ionized systems. The active sets of orbitals for the even and odd parity states were extended by layers to include orbitals with quantum numbers up to $n = 8$ and $l = 6$. Each layer of active orbitals were optimized separately in the EOL scheme, with the previous layers kept frozen. The MCDHF calculations were followed by RCI calculations, including mass-polarization, the Breit-interaction and leading QED effects. The number of CSFs in the final even and odd state expansions were approximately 640 000 and 630 000, respectively, distributed over the different J symmetries.

2.4. Labeling of states

In order to identify the computed states and match them against observations, the wave function expansions over jj -coupled CSFs were transformed to LSJ coupling (Gaigalas et al. 2003). In all tables of this paper the quantum states are labeled with the leading term of the LSJ -percentage composition. The labels

Table 2. Comparison of calculated and observed excitation energies in Ni XVII in cm^{-1} .

State	E_{RCI}	E_{NIST}	ΔE
$3s^2 \ ^1S_0$	0	0	
$3s3p \ ^3P_0^\circ$	264 431	264 431	0
$3s3p \ ^3P_1^\circ$	272 650	272 634	16
$3s3p \ ^3P_2^\circ$	293 707	293 686	21
$3s3p \ ^1P_1^\circ$	401 590	401 302	288
$3p^2 \ ^3P_0$	628 065	627 914	151
$3p^2 \ ^1D_2$	639 086	638 820	266
$3p^2 \ ^3P_1$	643 914	643 807	107
$3p^2 \ ^3P_2$	669 689	669 535	154
$3p^2 \ ^1S_0$	755 195	754 513	682
$3s3d \ ^3D_1$	771 391	771 268	123
$3s3d \ ^3D_2$	773 061	772 953	108
$3s3d \ ^3D_3$	775 691	775 567	124
$3s3d \ ^1D_2$	865 079	864 465	614
$3p3d \ ^3F_2^\circ$	1 054 212	1 053 937	275
$3p3d \ ^3F_3^\circ$	1 068 917	1 068 632	285
$3p3d \ ^1D_2^\circ$	1 081 412	1 081 126	286
$3p3d \ ^3F_4^\circ$	1 086 391	1 086 107	284
$3p3d \ ^3D_1^\circ$	1 115 712	1 115 521	191
$3p3d \ ^3D_{2A}^\circ$	1 118 619	1 118 392	227
$3p3d \ ^3D_3^\circ$	1 133 959	1 133 775	184
$3p3d \ ^3P_0^\circ$	1 136 049	1 135 732	317
$3p3d \ ^3P_1^\circ$	1 136 356	1 136 123	233
$3p3d \ ^3D_{2B}^\circ$	1 136 892	1 136 643	249
$3p3d \ ^1F_3^\circ$	1 209 617	1 209 017	600
$3p3d \ ^1P_1^\circ$	1 223 592	1 222 730	862
$3d^2 \ ^3F_2$	1 558 116	1 557 900?	216
$3d^2 \ ^3F_3$	1 560 874	1 560 490	384
$3d^2 \ ^3F_4$	1 564 179	1 563 822	357
$3d^2 \ ^1D_2$	1 595 636	1 594 821	815
$3d^2 \ ^3P_0$	1 598 455	1 597 400?	1055
$3d^2 \ ^3P_1$	1 599 485	1 598 889	596
$3d^2 \ ^1G_4$	1 602 182	1 601 404	778
$3d^2 \ ^3P_2$	1 602 280	1 601 729	551
$3d^2 \ ^1S_0$	1 692 810		

Notes. E_{RCI} are energies that include low-frequency Breit, vacuum polarization, and self-energy corrections from present calculations. E_{NIST} observed energies from the NIST Atomic Spectra Database (ver. 5.3; Kramida et al. 2015). Energies for all states in Ni XVII as well as energies for the ions Ca IX – As XXII and Kr XXV are available at the CDS.

obtained with this approach are, however, not unique and this is further discussed in the next section.

3. Results and discussion

3.1. Energies

In Table 1 we present the computed excitation energies for the 35 lowest levels in Fe XV belonging to the $3l3l'$ configurations as functions of the increasing active sets of orbitals labeled with the highest principal quantum number n of the orbitals in the set. For comparison, observed energies from the NIST Atomic Spectra Database (ver. 5.3; Kramida et al. 2015) are given as well. The relative differences between theory and observation are 0.122%, 0.49%, 0.050% and 0.041% for calculations based on

Table 3. Lifetimes in s. for Fe XV. τ_l and τ_v are lifetimes in length and velocity form, respectively.

State	RCI		MCHF-BP	CIV3	Expt.
	τ_l	τ_v	τ_l	τ_l	τ
3s 3p $^3P_1^o$	2.3266E-08	2.2036E-08	2.205E-08	2.571E-08	
3s 3p $^3P_2^o$	2.6328E-02	2.6328E-02	2.398E-02	2.478E-02	
3s 3p $^1P_1^o$	4.6507E-11	4.5922E-11	4.748E-11	4.339E-11	4.2E-11 \pm 0.3
3p ² 3P_0	5.8296E-11	5.7444E-11	5.804E-11	5.440E-11	
3p ² 1D_2	2.0553E-10	2.0145E-10	2.145E-10	2.235E-10	1.9E-10 \pm 0.2
3p ² 3P_1	5.4793E-11	5.4061E-11	5.422E-11	5.123E-11	
3p ² 3P_2	6.0296E-11	5.9589E-11	5.871E-11	5.497E-11	
3p ² 1S_0	5.1455E-11	5.1018E-11	5.093E-11	4.828E-11	6.3E-11 \pm 0.5
3s 3d 3D_1	4.2644E-11	4.2822E-11	4.184E-11	4.035E-11	
3s 3d 3D_2	4.4170E-11	4.4385E-11	4.343E-11	4.180E-11	
3s 3d 3D_3	4.6965E-11	4.7250E-11	4.608E-11	4.443E-11	
3s 3d 1D_2	2.4565E-11	2.4628E-11	2.425E-11	2.266E-11	3.6E-11 \pm 0.4
3p 3d $^3F_2^o$	1.6632E-10	1.6357E-10	1.604E-10	1.614E-10	
3p 3d $^3F_3^o$	1.9418E-10	1.9062E-10	1.934E-10	1.885E-10	
3p 3d $^1D_2^o$	5.6125E-11	5.6007E-11	5.675E-11	5.271E-11	
3p 3d $^3F_4^o$	1.8245E-10	1.7922E-10	1.815E-10	1.759E-10	
3p 3d $^3D_1^o$	2.6539E-11	2.6611E-11	2.630E-11	2.514E-11	
3p 3d $^3P_2^o$	3.0991E-11	3.1093E-11	3.097E-11	2.937E-11	
3p 3d $^3D_3^o$	2.5355E-11	2.5458E-11	2.522E-11	2.396E-11	
3p 3d $^3P_0^o$	3.2923E-11	3.3016E-11	3.270E-11	3.094E-11	
3p 3d $^3P_1^o$	3.0477E-11	3.0559E-11	3.034E-11	2.858E-11	
3p 3d $^3D_2^o$	2.8405E-11	2.8491E-11	2.818E-11	2.662E-11	
3p 3d $^1F_3^o$	2.3616E-11	2.3783E-11	2.315E-11	2.223E-11	
3p 3d $^1P_1^o$	2.6751E-11	2.6880E-11	2.650E-11	2.452E-11	
3d ² 3F_2	2.5833E-11	2.5991E-11	2.535E-11	2.463E-11	
3d ² 3F_3	2.6785E-11	2.6967E-11	2.620E-11	2.553E-11	
3d ² 3F_4	2.8018E-11	2.8231E-11	2.750E-11	2.671E-11	
3d ² 1D_2	2.2258E-11	2.2492E-11	2.206E-11	2.069E-11	
3d ² 3P_0	2.0753E-11	2.0973E-11	2.043E-11	1.948E-11	
3d ² 3P_1	2.1027E-11	2.1254E-11	2.061E-11	1.973E-11	
3d ² 1G_4	4.4681E-11	4.4948E-11	4.367E-11	4.368E-11	
3d ² 3P_2	2.1997E-11	2.2254E-11	2.151E-11	2.082E-11	
3d ² 1S_0	1.7296E-11	1.7588E-11	1.712E-11	1.581E-11	

Notes. RCI present calculations, MCHF-BP calculations by [Froese Fischer et al. \(2006\)](#), CIV3 calculations by [Aggarwal et al. \(2007\)](#) and Expt. beam-foil measurements by [Hutton et al. \(1988\)](#).

the expansion from the MR and the expansions from SD excitations to orbital sets with the highest principal quantum numbers $n = 6, 7, 8$. Looking more carefully at Table 1 it is seen that the triplet states show better convergence properties than the singlet states. For the singlet states the relative differences between theory and observation are 0.233%, 0.789%, 0.106% and 0.073% and the singlet states are not fully converged with respect to the orbital set. Adding a few orbital layers would improve the excitation energies, but would add to the total computation time. Differences in convergence rates are further analyzed and discussed in [Jönsson et al. \(2016\)](#). In Table 2 the computed excitation energies for Ni XVII (the full table for Ca IX – As XXII and Kr XXV is available at the CDS) based on the largest orbital set $n = 8$ are displayed together with observed energies from the NIST Atomic Spectra Database (ver. 5.3; [Kramida et al. 2015](#)). The differences between the computed and observed energies are

also given. For Kr XXV, excitation energies from accurate many-body perturbation calculations by [Si et al. \(2015\)](#) can be used for further comparisons.

The agreement between the computed excitation energies and the observed energies is generally very good, although the calculations give somewhat too high excitation energies for the states belonging to the $3l4l'$ and $3s5l$ configurations. For these states typical differences are between 1000 cm^{-1} and 2000 cm^{-1} , which translates to relative differences of theory and observation between 0.05% and 0.1%. The difference between calculations and observations can be explained by the fact that the current calculations extend to many configurations and that the calculations are not fully converged with respect to the orbital basis. The difference is also due to the fact that core-core electron correlation were neglected, the effect of which is to lower the energies of the higher lying states. There are many states for which theory

and observations do not agree at all. An example is $3s4d\ ^1D_2$, where the difference is -4488 cm^{-1} in Sc X and 6498 cm^{-1} in Ti XI. These disagreements may be due to difficulties in identification or labeling of levels derived from observed data. The present data are useful in validating the identification of levels.

As for most calculations involving states of many configurations there are labeling problems (Jönsson et al. 2013a). States are often labeled by the leading term of the wave function LSJ -percentage composition. For closely lying interacting states with the same J , the leading term can be the same. To resolve this the label can be based on more terms of the composition. A simpler solution is to add an extra index to the leading term of the composition. We choose the latter solution. For example, the two $J = 3$ states in Fe XV at $2\,316\,401\text{ cm}^{-1}$ and $2\,333\,084\text{ cm}^{-1}$ both have the leading term $3p4d\ ^3D_3$. These two states were labeled $3p4d\ ^3D_{3a}$ and $3p4d\ ^3D_{3b}$, respectively. It is important to realize that the wave function LSJ -percentage composition depends on the details of the calculation, and thus two calculations can have slight differences in compositions leading to differences in labels.

3.2. Lifetimes

Lifetimes of the excited states were calculated from E1 and M1 transition rates. The contributions to the lifetimes from E2 and higher multipoles are negligible. In Table 3 the present lifetimes for the 84 lowest states in Fe XV in length and velocity form are compared with lifetimes from the multiconfiguration Hartree-Fock Breit-Pauli (MCHF-BP) calculations by Froese Fischer et al. (2006) and with the CIV3 calculations by Aggarwal et al. (2007). Included in the table are also lifetimes from beam-foil measurements by Hutton et al. (1988).

The average relative difference between the lifetimes in the length and velocity forms from the present calculation is less than 0.52%, which is highly satisfactory. This difference can be seen as an internal validation of the accuracy. The differences between the present lifetimes in the length form and the lifetimes by Froese Fischer et al. (2006) and Aggarwal et al. (2007) are 1.37% and 4.45%, respectively. Comparing theoretical and experimental lifetimes we see that they do not agree very well. This may be due to large uncertainties in the beam-foil measurements as discussed in Zou et al. (1999). In Table 4 the computed lifetimes in length form and the uncertainty estimators dT are displayed for Fe XV (the full table for Ca IX – As XXII and Kr XXV is available at the CDS) based on the largest orbital set $n = 8$.

3.3. Oscillator strengths and transition rates

In Table 5 the present oscillator strengths in the length form for selected transitions in Fe XV are compared with values from the MCHF-BP calculations by Froese Fischer et al. (2006) and with values from the CIV3 and MCDHF calculations by Aggarwal et al. (2007). Values from the present calculations and the MCHF-BP calculations agree to within 1.53%. The agreement with the CIV3 and MCDHF calculations by Aggarwal et al. (2007) is 8.42% and 6.50%, respectively. The results of the comparisons are explained by the fact that the RCI and MCHF-BP calculations include more electron correlation effects than do the CIV3 and MCDHF calculations. Due to the neglected electron correlation two the latter calculations are believed to be somewhat less accurate.

Table 4. Lifetimes in s for Fe XV.

State	τ	dT
$3s3p\ ^3P_1^o$	2.3266E-08	0.0529
$3s3p\ ^3P_2^o$	2.6328E-02	0.0000
$3s3p\ ^1P_1^o$	4.6507E-11	0.0126
$3p^2\ ^3P_0$	5.8296E-11	0.0146
$3p^2\ ^1D_2$	2.0553E-10	0.0198
$3p^2\ ^3P_1$	5.4793E-11	0.0133
$3p^2\ ^3P_2$	6.0296E-11	0.0117
$3p^2\ ^1S_0$	5.1455E-11	0.0085
$3s3d\ ^3D_1$	4.2644E-11	0.0042
$3s3d\ ^3D_2$	4.4170E-11	0.0048
$3s3d\ ^3D_3$	4.6965E-11	0.0060
$3s3d\ ^1D_2$	2.4565E-11	0.0026
$3p3d\ ^3F_2^o$	1.6632E-10	0.0165
$3p3d\ ^3F_3^o$	1.9418E-10	0.0183
$3p3d\ ^1D_2^o$	5.6125E-11	0.0021
$3p3d\ ^3F_4^o$	1.8245E-10	0.0177
$3p3d\ ^3D_1^o$	2.6539E-11	0.0027
$3p3d\ ^3P_2^o$	3.0991E-11	0.0033
$3p3d\ ^3D_3^o$	2.5355E-11	0.0040
$3p3d\ ^3P_0^o$	3.2923E-11	0.0028
$3p3d\ ^3P_1^o$	3.0477E-11	0.0027
$3p3d\ ^3D_2^o$	2.8405E-11	0.0030
$3p3d\ ^1F_3^o$	2.3616E-11	0.0071
$3p3d\ ^1P_1^o$	2.6751E-11	0.0048
$3d^2\ ^3F_2$	2.5833E-11	0.0061
$3d^2\ ^3F_3$	2.6785E-11	0.0067
$3d^2\ ^3F_4$	2.8018E-11	0.0076
$3d^2\ ^1D_2$	2.2258E-11	0.0104
$3d^2\ ^3P_0$	2.0753E-11	0.0105
$3d^2\ ^3P_1$	2.1027E-11	0.0107
$3d^2\ ^1G_4$	4.4681E-11	0.0059
$3d^2\ ^3P_2$	2.1997E-11	0.0116
$3d^2\ ^1S_0$	1.7296E-11	0.0166

Notes. τ is lifetime in length form and dT is the uncertainty estimator given by Eq. (2). Lifetimes for all states in Fe XV as well as lifetimes for the ions Ca IX – As XXII and Kr XXV are available at the CDS.

In Table 6 the transition energies, wavelengths, transition rates A , and weighted oscillator strengths gf are given for Fe XV (the full table for Ca IX – As XXII and Kr XXV is available at the CDS). All E1 and M1 transitions with rates A larger than 10^4 s^{-1} are displayed. Transition data are also given for transitions with rates A greater than a fraction 10^{-4} of the sum of the A -values for transitions from the upper level. For the E1 transitions also the uncertainty indicator dA is given. For most of the stronger E1 transitions dA is below 1%. For the weaker transitions the situation is somewhat different. While many of the weaker transitions have dA in the range from a few percent up to 10% there are also many transitions for which dA is considerably larger. These transitions are often so called two-electron one-photon transitions for which the configurations involved in the transitions differ by two electrons. For two-electron one-photon transitions the rate between two states is determined, not from the major CSFs that define the label, but from other CSFs of the wave function expansion, often CSFs that are part of the MR set. We take the $3s5d\ ^3D_2 - 3p4s\ ^3P_2^o$ transition in Ca IX at 499.614 \AA as an example. The rate is $A = 1.716 \times 10^6\text{ s}^{-1}$ and $dA = 0.166$.

Table 5. Oscillator strengths f for selected transitions in Fe XV.

Upper	Lower	f_{RCI}	$f_{\text{MCHF-BP}}$	f_{CIV3}	f_{MCDF}
3s ² 1S ₀	3s3p 3P ₁	3.365E-03	3.584E-03	3.003E-03	3.069E-03
3s ² 1S ₀	3s3p 1P ₁	7.797E-01	7.738E-01	8.044E-01	8.147E-01
3s ² 1S ₀	3s4p 1P ₁	2.941E-01	2.789E-01	2.634E-01	2.966E-01
3s3p 3P ₀	3p ² 3P ₁	2.743E-01	2.753E-01	2.838E-01	2.874E-01
3s3p 3P ₀	3s3d 3D ₁	3.026E-01	3.049E-01	3.117E-01	3.149E-01
3s3p 3P ₁	3p ² 3P ₀	8.609E-02	8.618E-02	8.931E-02	9.037E-02
3s3p 3P ₁	3p ² 1D ₂	2.960E-02	2.799E-02	2.229E-02	2.624E-02
3s3p 3P ₁	3p ² 3P ₁	6.697E-02	6.715E-02	6.927E-02	7.026E-02
3s3p 3P ₁	3p ² 3P ₂	8.802E-02	9.016E-02	9.953E-02	9.684E-02
3s3p 3P ₁	3s3d 3D ₁	7.392E-02	7.442E-02	7.648E-02	7.693E-02
3s3p 3P ₁	3s3d 3D ₂	2.236E-01	2.251E-01	2.305E-01	2.327E-01
3s3p 3P ₂	3p ² 1D ₂	3.471E-02	3.171E-02	2.526E-02	3.055E-02
3s3p 3P ₂	3p ² 3P ₁	6.375E-02	6.396E-02	6.607E-02	6.689E-02
3s3p 3P ₂	3p ² 3P ₂	1.661E-01	1.698E-01	1.826E-01	1.800E-01
3s3p 3P ₂	3s3d 3D ₁	2.863E-03	2.885E-03	2.982E-03	2.976E-03
3s3p 3P ₂	3s3d 3D ₂	4.344E-02	4.374E-02	4.508E-02	4.515E-02
3s3p 3P ₂	3s3d 3D ₃	2.442E-01	2.460E-01	2.521E-01	2.540E-01
3s3p 1P ₁	3p ² 1D ₂	8.590E-02	8.832E-02	9.024E-02	8.799E-02
3s3p 1P ₁	3p ² 1S ₀	1.006E-01	1.010E-01	1.052E-01	1.062E-01
3s3p 1P ₁	3s3d 1D ₂	5.978E-01	6.000E-01	6.323E-01	6.338E-01
3p ² 1D ₂	3p3d 1D ₂	1.366E-01	1.355E-01	1.577E-01	1.503E-01
3p ² 1D ₂	3p3d 1P ₁	1.215E-03		1.723E-03	1.512E-03
3p ² 3P ₁	3p3d 3D ₁	3.562E-02	3.661E-02	3.916E-02	3.549E-02
3p ² 3P ₁	3p3d 3P ₀	5.365E-02	5.390E-02	5.604E-02	5.622E-02
3p ² 3P ₁	3p3d 3P ₁	1.166E-01	1.163E-01	1.184E-01	1.238E-01
3p ² 3P ₂	3p3d 3D ₁	1.474E-03		1.383E-03	1.785E-03
3p ² 3P ₂	3p3d 3D ₃	2.797E-01	2.866E-01	3.137E-01	3.061E-01
3p ² 3P ₂	3p3d 3P ₁	3.411E-02	3.508E-02	3.822E-02	3.679E-02
3p ² 1S ₀	3p3d 1P ₁	6.313E-01	6.348E-01	6.624E-01	6.688E-01
3s3d 3D ₁	3p3d 3F ₂	1.202E-01	1.168E-01	1.278E-01	1.272E-01
3s3d 3D ₁	3p3d 3D ₁	3.176E-02	3.242E-02	3.536E-02	3.171E-02
3s3d 3D ₁	3p3d 3P ₀	5.153E-02	5.147E-02	5.334E-02	5.494E-02
3s3d 3D ₁	3p3d 3P ₁	1.096E-01	1.087E-01	1.113E-01	1.176E-01
3s3d 3D ₂	3p3d 3F ₂	1.973E-02	1.934E-02	2.037E-02	2.045E-02
3s3d 3D ₂	3p3d 3F ₃	1.235E-01	1.231E-01		
3s3d 3D ₂	3p3d 3D ₁	6.188E-02	6.122E-02		
3s3d 3D ₂	3p3d 3D ₃	3.705E-02	3.759E-02		
3s3d 3D ₂	3p3d 3P ₁	2.463E-02	2.513E-02	2.698E-02	2.540E-02
3s3d 3D ₃	3p3d 3F ₂	2.106E-04		2.497E-04	2.333E-04
3s3d 3D ₃	3p3d 3F ₃	2.045E-02	2.071E-02		
3s3d 3D ₃	3p3d 3F ₄	1.466E-01	1.469E-01		
3s3d 1D ₂	3p3d 1D ₂	3.075E-02	3.018E-02	3.081E-02	3.079E-02
3s3d 1D ₂	3p3d 1F ₃	3.847E-01	3.857E-01		
3s3d 1D ₂	3p3d 1P ₁	1.090E-01	1.091E-01		
3p3d 3F ₄	3p4f 3G ₅	7.892E-01	7.878E-01		
3p3d 3P ₀	3p4f 3D ₁	9.360E-01	9.327E-01		
3p3d 1F ₃	3p4f 1G ₄	7.104E-01	7.128E-01		

Notes. f_{RCI} present work in length form, $f_{\text{MCHF-BP}}$ calculations by [Froese Fischer et al. \(2006\)](#), f_{CIV3} and f_{MCDF} are calculations by [Aggarwal et al. \(2007\)](#).

Table 6. Transition data for Fe XV.

Upper	Lower	EM	ΔE (cm ⁻¹)	λ (Å)	A (s ⁻¹)	gf	dA
3d4f ³ P ₁ ^o	3s ² ¹ S ₀	E1	2 811 468	35.569	3.455E+06	1.966E-06	0.166
3d4f ³ D ₁ ^o	3s ² ¹ S ₀	E1	2 807 002	35.625	6.076E+05	3.468E-07	0.052
3p5s ³ P ₁ ^o	3s ² ¹ S ₀	E1	2 797 247	35.749	3.125E+07	1.796E-05	0.195
3d4p ¹ P ₁ ^o	3s ² ¹ S ₀	E1	2 605 145	38.386	1.939E+10	1.285E-02	0.020
3d4p ³ P ₁ ^o	3s ² ¹ S ₀	E1	2 585 242	38.681	1.924E+09	1.295E-03	0.018
3s5p ¹ P ₁ ^o	3s ² ¹ S ₀	E1	2 571 834	38.883	9.560E+10	6.500E-02	0.016
3s5p ³ P ₁ ^o	3s ² ¹ S ₀	E1	2 568 791	38.929	3.266E+10	2.226E-02	0.016
3d4p ³ D ₁ ^o	3s ² ¹ S ₀	E1	2 567 301	38.951	4.413E+10	3.011E-02	0.016
3d4d ¹ S ₀	3s3p ³ P ₁ ^o	E1	2 539 607	39.376	4.010E+08	9.321E-05	0.019
3d4d ³ P ₁	3s3p ³ P ₀ ^o	E1	2 512 797	39.796	5.635E+08	4.014E-04	0.022
3d4d ³ P ₂	3s3p ³ P ₁ ^o	E1	2 508 140	39.870	2.885E+08	3.438E-04	0.023
3d4d ³ P ₁	3s3p ³ P ₁ ^o	E1	2 506 958	39.889	4.049E+08	2.897E-04	0.022
3d4d ³ P ₀	3s3p ³ P ₁ ^o	E1	2 506 354	39.899	1.857E+09	4.431E-04	0.021
3d4d ¹ D ₂	3s3p ³ P ₁ ^o	E1	2 504 194	39.933	1.366E+08	1.633E-04	0.019
3d4d ³ P ₂	3s3p ³ P ₂ ^o	E1	2 493 979	40.097	1.003E+09	1.209E-03	0.023
3d4d ³ P ₁	3s3p ³ P ₂ ^o	E1	2 492 797	40.116	7.030E+08	5.088E-04	0.021
3d4d ¹ D ₂	3s3p ³ P ₂ ^o	E1	2 490 033	40.160	1.344E+08	1.625E-04	0.019
3d4d ³ S ₁	3s3p ³ P ₀ ^o	E1	2 489 346	40.171	2.967E+08	2.153E-04	0.017
3d4d ³ F ₂	3s3p ³ P ₁ ^o	E1	2 488 424	40.186	1.772E+06	2.145E-06	0.005
3d4d ³ S ₁	3s3p ³ P ₁ ^o	E1	2 483 506	40.266	8.205E+08	5.983E-04	0.018
3d4d ¹ P ₁	3s3p ³ P ₀ ^o	E1	2 477 984	40.355	1.313E+08	9.616E-05	0.007
3d4d ³ F ₃	3s3p ³ P ₂ ^o	E1	2 475 569	40.395	1.255E+06	2.150E-06	0.003
3d4d ³ F ₂	3s3p ³ P ₂ ^o	E1	2 474 263	40.416	5.594E+04	6.849E-08	0.019
3d4d ¹ P ₁	3s3p ³ P ₁ ^o	E1	2 472 144	40.451	2.789E+06	2.053E-06	0.076
3d4d ³ D ₁	3s3p ³ P ₀ ^o	E1	2 472 143	40.451	1.154E+09	8.489E-04	0.005
3d4d ³ S ₁	3s3p ³ P ₂ ^o	E1	2 469 345	40.497	1.145E+09	8.444E-04	0.024
3d4d ³ D ₂	3s3p ³ P ₁ ^o	E1	2 467 549	40.526	1.659E+09	2.043E-03	0.005
3d4d ³ D ₁	3s3p ³ P ₁ ^o	E1	2 466 303	40.547	9.922E+08	7.337E-04	0.006
3d4d ¹ P ₁	3s3p ³ P ₂ ^o	E1	2 457 983	40.684	2.782E+07	2.071E-05	0.016
3d4d ³ G ₃	3s3p ³ P ₂ ^o	E1	2 456 693	40.705	7.310E+06	1.271E-05	0.006
3d4d ³ D ₃	3s3p ³ P ₂ ^o	E1	2 454 806	40.736	2.012E+09	3.505E-03	0.006
3d4d ³ D ₂	3s3p ³ P ₂ ^o	E1	2 453 388	40.760	5.027E+08	6.260E-04	0.007
3d4d ³ D ₁	3s3p ³ P ₂ ^o	E1	2 452 142	40.781	4.270E+07	3.194E-05	0.008
3d4d ¹ F ₃	3s3p ³ P ₂ ^o	E1	2 447 773	40.853	5.584E+07	9.780E-05	0.005
3d4d ¹ S ₀	3s3p ¹ P ₁ ^o	E1	2 427 106	41.201	1.657E+10	4.216E-03	0.028

Notes. ΔE is transition energy in cm⁻¹, λ is transition wavelength in Å, A is transition rate in s⁻¹, gf is weighted oscillator strength, dA is uncertainty estimator given by Eq. (2). Data for all transitions in Fe XV as well as for transitions in Ca IX – As XXII and Kr XXV are available at the CDS.

In LSJ coupling the major contributors to the states are

$$\begin{aligned} &0.75964323 \quad 3s5d \ ^3D_2 \\ &-0.63064515 \quad 3p4f \ ^3D_2 \\ &0.06792502 \quad 3s5d \ ^1D_2 \\ &0.06676172 \quad 3p4f \ ^3F_2 \\ &-0.06265593 \quad 3p4f \ ^1D_2 \end{aligned}$$

and

$$\begin{aligned} &0.99191041 \quad 3p4s \ ^3P_2^o \\ &0.07887890 \quad 3s4p \ ^3P_2^o \\ &0.07366793 \quad 3d4p \ ^3P_2^o \\ &0.04500217 \quad 3p4d \ ^3P_2^o. \end{aligned}$$

Due to the selection rules of the transition operator, contributions to A are zero from the two dominating CSFs of the even state to

the dominating CSF of the odd state. The transition rate A is instead determined by contributions from different combinations of the remaining CSFs. The lack of contributions from the dominating CSFs together with many smaller and canceling contributions from the remaining CSFs often make the two-electron one-photon transitions weak and with large values of dA. Although important and challenging from a theoretical point of view, these weak transitions have little practical importance in modeling applications.

3.4. Summary and conclusions

MCDHF and subsequent RCI calculations were performed for states of the $3/3'$, $3/4'$ and $3s/5l$ configurations in the Mg-like ions Ca IX – As XXII and Kr XXV and excitation energies,

lifetimes, and transition data are presented for all ions. Excitation energies from the RCI calculations are in very good agreement with available observations for the lower states. For the higher states the calculated excitations energies are 1000 cm^{-1} – 2000 cm^{-1} larger than energies from observations. There are also anomalous differences, either positive or negative, between calculations and observations due to misidentifications. One example is the $3p4f$ configuration in Cu XVIII. Here the difference between calculations and observations are $22\,083\text{ cm}^{-1}$ and 1432 cm^{-1} for $3p4f\ ^3D_3$ and $3p4f\ ^3D_2$, respectively. The former difference indicates a misidentification of observed data.

Lifetimes were internally validated by comparing values in length and velocity form. Lifetimes in the two forms differ in average at the 0.5% level. Systematic comparisons with the MCHF-BP calculations by Froese Fischer et al. (2006) showed that lifetimes from these two calculations differ on average only by 1.5%. Also for the oscillator strengths the present calculations showed good consistency with the MCHF-BP with an average relative difference of 1.5% for selected transitions in Fe XV. Uncertainties of the transition rates are estimated by dA , as suggested by Ekman et al. (2014). For most of the stronger transitions, dA is below 1%. The transition rates for many of the weak two-electron one-photon transitions are highly uncertain, as indicated by large values of dA .

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