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Fine-structure energy levels, oscillator strengths and lifetimes in Mg-like chromium*

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Abstract. Excitation energies from ground state for 86 fine-structure levels as well as oscillator strengths and radiative decay rates for all fine-structure transitions among the levels of the terms $(1s^22s^22p^6)3s^2(^1\mathrm{S})$, $3s3p(^{1,3}\mathrm{P}^o)$, $3s3d(^{1,3}\mathrm{D})$, $3s4s(^{1,3}\mathrm{S})$, $3s4p(^{1,3}\mathrm{P}^o)$, $3s4d(^{1,3}\mathrm{D})$, $3s4f(^{1,3}\mathrm{F}^o)$, $3p^2(^1\mathrm{S}, {}^3\mathrm{P}, {}^1\mathrm{D})$, $3p3d(^{1,3}\mathrm{P}^o, {}^{1,3}\mathrm{D}^o, {}^{1,3}\mathrm{F}^o)$, $3p4s(^{1,3}\mathrm{P}^o)$, $3p4p(^{1,3}\mathrm{S}, {}^{1,3}\mathrm{P}, {}^{1,3}\mathrm{D})$, $3p4d(^{1,3}\mathrm{P}^o, {}^{1,3}\mathrm{D}^o, {}^{1,3}\mathrm{F}^o)$, $3p4f(^{1,3}\mathrm{D}, {}^{1,3}\mathrm{F}, {}^{1,3}\mathrm{G})$ and $3d^2(^1\mathrm{S}, {}^3\mathrm{P}, {}^1\mathrm{D}, {}^3\mathrm{F}, {}^1\mathrm{G})$ of Cr XIII are calculated using extensive configuration-interaction (CI) wave functions obtained with the CIV3 computer code of Hibbert. The important relativistic effects in intermediate coupling are included through the Breit-Pauli approximation via spin-orbit, spin-other-orbit, spin-spin, Darwin and mass correction terms. Small adjustments to the diagonal elements of the Hamiltonian matrices have been made. The mixing among several fine-structure levels is found to be very strong. Our excitation energies, including their ordering, are in excellent agreement (better than 0.5%) with the available experimental results. From our transition probabilities, we have also calculated radiative lifetimes of some fine-structure levels. Our calculated lifetime for the longer-lived level $3s3p(^3\mathrm{P}_1)$ is found to be in excellent agreement with the experimental result of Curtis compared to other theoretical calculations.

PACS. 32.10.Fn Fine and hyperfine structure – 32.70.Cs Oscillator strengths, lifetimes, transition moments – 95.30.Ky Atomic and molecular data, spectra, and spectral parameters (opacities, rotation constants, line identification, oscillator strengths, gf values, transition probabilities, etc.)

1 Introduction

Highly ionized species of the cosmically abundant metals such as Na, Mg, Si, Fe, and Ni radiate in the UV and X-ray band [1], and stellar coronal spectra are rich in emission lines from their high ionization states [2]. Also, their lower charge states produce X-rays through fluorescence following inner-shell ionization. In particular, the accurate determination of gas-phase abundances of species such as Mg and Si is very difficult [3]. The most important lines for obtaining reliable interstellar column densities for abundant elements, such as Mg, are the weak lines with small oscillator strengths [4]. Single- and multiple-charged positive ions are important emitters or serve as useful temperature and density diagnostics in various astrophysical objects (stars, quasars, planetary nebulae, etc.).

Elements in the Mg isoelectronic sequence are astrophysically abundant and accurate atomic data such as absorption oscillator strengths and transition probabilities are needed for the interpretation of accurate observational data. These atomic data are also useful for estimating the energy loss through impurity ions in fusion plasmas, and for diagnostic and modeling of the plasmas.

Most of the experimental and theoretical atomic data of energy levels, oscillator strengths, transition probabilities and lifetimes for ions of the Mg isoelectronic sequence, available in the literature, are limited to a few transitions among the terms belonging to the $3s^2$, $3s3p$, $3p^2$, and $3s3d$ configurations or lack accuracy. Fawcett [5] has calculated the wavelengths (λ) and weighted oscillator strengths ($\omega_i f_{ij}$) within the third shell for some ions in the Mg-like isoelectronic sequence. Tayal [6] calculated the excitation energies and oscillator strengths for electric-dipole allowed and intercombination transitions among the low-lying states in Ar VII, Ca IX and Fe XV. Chou et al. [7] evaluated relativistic excitation energies and oscillator strengths for the intercombination and resonance transitions in Mg-like ions using the multiconfiguration relativistic random-phase approximation including excitation channels from core electrons. Butler et al. [8] calculated energies and oscillator strengths for some transitions in a number of Mg-like ions using a modified *R*-matrix program. Stanek et al. [9] determined relativistic multiconfiguration Dirac-Fock (MCDF) transition energies and oscillator strengths in an optical level scheme for both

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[*] Table 3 with all the calculated lines is available with the first author.

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the spin-allowed and spin-forbidden $3s^2(^1\mathrm{S}_0)$–$3s3p(^1\mathrm{P}_1, {}^3\mathrm{P}_1)$ transitions in the Mg isoelectronic sequence and compared their data for the former with those of Wiese [10] and Chou et al. [7]. Jönsson and Froese-Fischer [11] carried out accurate multi-configuration Dirac-Fock calculations of transition probabilities, focusing on the $3s^2(^1\mathrm{S}_0)$–$3s3p(^1\mathrm{P}_1, {}^3\mathrm{P}_{1,2})$ transitions in the Mg isoelectronic sequence. *B*-spline basis techniques have been used by Chen and Cheng [12] to investigate transition energies in Mg-like ions. Deb and Msezane [13] and Deb et al. [14] studied level energies in Mg-like Fe XV using the program CIV3. Almaraz et al. [15] have performed extensive CIV3 calculations to investigate configuration mixing among the levels involved in the $3s^2(^1\mathrm{S}_0)$–$3snp(^{1,3}\mathrm{P})$ ($n = 3$–5) transitions in Mg-like ions. They also employed relativistic quantum defect orbital (RQDO) and MCDF methods in their investigations. Relativistic Many-Body Perturbation Theory (MBPT) has been used by Safronova et al. [16] to obtain excitation energies, transition probabilities and lifetimes for the electric dipole transitions in Mg-like ions ($Z = 13$–100). Zou and Froese-Fischer [17] applied multi-configuration Dirac-Fock method to the forbidden transitions between $3s^2(^1\mathrm{S}_0)$ and $3s3p(^1\mathrm{P}_1, {}^3\mathrm{P}_{0,1,2})$ states for Mg-like ions. Tachiev and Froese Fischer [18] calculated the energy levels and lifetimes in Cr XIII using multi-configuration Hartree-Fock (MCHF) wavefunctions and also reported the oscillator strengths for few low-lying states. Radiative lifetimes and oscillator strengths in Mg-like K VIII have been calculated by Biémont et al. [19] using relativistic HF and MCDF methods. Das et al. [20] studied using program CIV3 electric-dipole allowed and intercombination transitions in Mg-like K VIII and Ti XI within the $n = 3$ and $n = 4$ complexes and also obtained the lifetimes of some relatively longer-lived levels. Gupta and coworkers [21–23] have recently reported results for excitation energies, oscillator strengths, transition probabilities and lifetimes for transitions in several Mg-like ions using configuration-interaction code [24] and the Breit-Pauli Hamiltonian [25]. The energy spectra of Mg-like Cr XIII have been compiled by Shirai et al. [26].

In our calculation we used the Slater-type orbitals in program CIV3 [24] to construct the large configuration-interaction (CI) wavefunctions. The important relativistic effects in intermediate coupling are incorporated by means of the Breit-Pauli Hamiltonian which consists of the non-relativistic term plus the one-body mass correction, Darwin term, and spin-orbit, spin-other-orbit, and spin-spin operators [25]. These extensive CI wavefunctions in intermediate coupling schemes are then used to calculate the excitation energies, oscillator strengths, and transition probabilities for electric-dipole-allowed and inter-combination transitions among the $(1s^2 2s^2 2p^6)3s^2(^1\mathrm{S})$, $3s3p(^{1,3}\mathrm{P^o})$, $3s3d(^{1,3}\mathrm{D})$, $3s4s(^{1,3}\mathrm{S})$, $3s4p(^{1,3}\mathrm{P^o})$, $3s4d(^{1,3}\mathrm{D})$, $3s4f(^{1,3}\mathrm{F^o})$, $3p^2(^1\mathrm{S}, {}^3\mathrm{P}, {}^1\mathrm{D})$, $3p3d(^{1,3}\mathrm{P^o}, {}^{1,3}\mathrm{D^o}, {}^{1,3}\mathrm{F^o})$, $3p4s(^{1,3}\mathrm{P^o})$, $3p4p(^{1,3}\mathrm{S}, {}^{1,3}\mathrm{P}, {}^{1,3}\mathrm{D})$, $3p4d(^{1,3}\mathrm{P^o}, {}^{1,3}\mathrm{D^o}, {}^{1,3}\mathrm{F^o})$, $3p4f(^{1,3}\mathrm{D}, {}^{1,3}\mathrm{F}, {}^{1,3}\mathrm{G})$ and $3d^2(^1\mathrm{S}, {}^3\mathrm{P}, {}^1\mathrm{D}, {}^3\mathrm{F}, {}^1\mathrm{G})$ states of Cr XIII, mainly to complete the void in the existing data and provide many additional new and accurate data for various optically allowed and intercombination transitions. From our transition probabilities we have also calculated the radiative lifetimes of all fine-structure levels. We have investigated the effects of electron correlations on our calculated data, particularly on the intercombination transitions, by including orbitals with up to $n = 5$ quantum number. We considered up to two electron excitations from the valence electrons of the basic configurations and included 322 configurations to ensure convergence. These configurations represent all major internal, semi-internal and all-external electron correlation effects [27]. Here we have obtained data for many dipole-allowed and intercombination transitions. The importance of the latter is that they are forbidden in the pure LS coupling scheme. However, they become allowed in the intermediate coupling through the spin-orbit mixing of different LS symmetries with the same total angular momentum values, J.

2 Choice of radial wavefunctions and configurations

The 47 LS states belonging to the $(1s^2 2s^2 2p^6)3s^2$, $3s3p$, $3s3d$, $3s4s$, $3s4p$, $3s4d$, $3s4f$, $3p^2$, $3p3d$, $3p4s$, $3p4p$, $3p4d$, $3p4f$ and $3d^2$ configurations of Cr XIII give rise to 87 fine-structure levels corresponding to various J values — see Table 2. The wave functions describing LS atomic states are obtained using the CIV3 code of Hibbert [24], and are written in the form:

$$\Psi(LS) = \sum_{i}^{M} a_{i,LS} \Phi_i(\alpha_i LS) \tag{1}$$

in which the single-configuration functions $\{\Phi_i\}$ are eigenfunctions of the total orbital and spin angular momenta (L, and S common to all M configurations), and are constructed from one electron orbitals of the form

$$u(\mathbf{r}, m_s) = \frac{1}{r} P_{nl}(r) Y_l^{ml}(\theta, \phi) \chi(m_s). \tag{2}$$

The radial function $P_{nl}(r)$ can be expanded analytically as sums of normalized Slater type orbital:

$$P_{nl}(r) = \sum_{j=1}^{k} C_j N_j r^{p_i} \exp(-\xi_i r) \tag{3}$$

where

$$N_j = \left\{ \frac{(2\xi_i)^{2p_i+1}}{(2\xi)!} \right\}^{1/2} \tag{4}$$

and

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) dr = \delta_{nn'}. \tag{5}$$

According to the Hylleraas-Undheim theorem, the parameters in (3) can be optimized on any one of the eigenvalues of the Hamiltonian matrix $\langle \Phi_i | \mathrm{H} | \Phi_j \rangle$. These eigenvalues form upper bounds to the energies of corresponding states with the $\{a_i\}$ in (1) being the components

Table 1. Radial function parameters for optimized orbitals of Cr XIII.

Orbitals	C_i	p_i	ξ_i
$3p$	0.4923495	2	9.9213062
	–1.1007825	3	4.7120013
$3d$	1.0000000	3	4.8928579
$4s$	0.1206364	1	18.2101779
	–0.5808871	2	7.6281820
	2.1095159	3	4.2415785
	–2.2810690	4	3.7178873
$4p$	0.3382346	2	9.6229656
	–2.5506005	3	3.5489105
	2.9661067	4	3.5666899
$4d$	0.7541706	3	5.0620691
	–1.2305529	4	3.1242659
$4f$	1.0000000	4	3.3389110
$5s$	1.3369142	1	3.9482551
	–9.2048668	2	4.0522475
	24.1818521	3	4.0550887
	–28.3872545	4	4.0430339
	12.4766737	5	4.0444450
$5p$	16.6084981	2	3.1422144
	–106.5072625	3	4.3636434
	183.5908783	4	5.5677539
	–94.0727653	5	6.7635544
$5d$	1.4232442	3	10.0180892
	–3.0514330	4	5.3589302
	2.3572971	5	5.4560799
$5f$	3.0563438	4	4.2376885
	–2.8781691	5	4.2051573
$5g$	1.0000000	5	5.9928770

of the corresponding eigenvector, and satisfying the condition that $\sum a_i^2 = 1$.

In our calculation we used the 15 orthogonal one-electron orbitals: $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, $4s$, $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, $5f$, and $5g$. The $1s$, $2s$, $2p$ and 3s radial functions are chosen as the Hartree-Fock (HF) functions of the ground state $(1s^2 2s^2 2p^6)$ $3s^2$ (^{1}S) of Cr XIII given by Clementi and Roetti [28]. The $3p$, $4s$, $4p$, $4d$ and $4f$ functions are chosen as spectroscopic type and are optimized, using the CIV3 program of Hibbert [24], on the excited states $3s3p(^1\mathrm{P^o})$, $3s4s(^3\mathrm{S})$, $3s4p(^3\mathrm{P^o})$, $3s4d(^3\mathrm{D})$, and $3s4f(^3\mathrm{F^o})$, respectively. In order to represent the strong interaction between the $3s3d$ (^{1}D) and $3p^2$ (^{1}D) configurations correctly, the $3d$ orbital is chosen as a correlation type [29] and optimized on the $3p^2(^1\mathrm{D})$ level. In order to represent all the energy levels by a single set of orthogonal functions, the remaining $5s$, $5p$, $5d$, $5f$, and $5g$ orbitals are chosen as correlation-type and optimized on the excited states to minimize the energies of the $3p^2$ (^{1}S), $3s3p$ ($^1\mathrm{P^o}$), $3s3d$ (^{1}D), $3p3d$ ($^3\mathrm{D^o}$) and $3p3d$ ($^1\mathrm{F^o}$) states, respectively. In all cases we chose $K = n - l$ so that the coefficients C_i are uniquely specified by the orthogonality condition on P_{nl} [24]. The parameters of the optimized radial functions are displayed in Table 1.

In this calculation we considered up to two-electron excitations from the valence shells. We have retained all configurations within the $n = 5$ complex that had weights $\geqslant 0.001$ for the states that mixed strongly, and $\geqslant 0.002$ for the remaining states. The contribution from the higher orbitals with the $n = 6$ and 7 complexes was also assessed, and was found to be insignificant.

The J-dependent CI wave functions are constructed by using expansions of the form [25]

$$\Psi_i(JM_J) = \sum_{j=1}^{K} b_{ij} \phi_j(\alpha_j L_j S_j J M_J), \tag{6}$$

where each of the K single-configuration functions ϕ_j is constructed from one-electron functions and α_j defines the coupling of the orbital L_j and the spin S_j angular momenta to give the total angular momentum J. The mixing coefficients b_{ij} are the eigenvector components of the Hamiltonian matrix $\langle \phi_i | H | \phi_j \rangle$ with the basis ϕ_j [25]. The Hamiltonian is represented by the non-relativistic electrostatic interactions plus the Breit-Pauli terms such as one-body mass correction, Darwin term, and spin-orbit, spin-other-orbit, and spin-spin operators. The complete description of the individual terms of the Breit-Pauli Hamiltonian can be found in the book of Froese Fischer et al. [30], Chapter 7 and references therein. The details of the implementation of the Breit-Pauli Hamiltonian in program CIV3 are given in Glass and Hibbert [25]. The inclusion of mass correction and Darwin terms shifts the energy of a configuration as a whole while the spin-orbit and spin-other-orbit terms cause the fine-structure splitting. The spin-spin term contributes both to the energy of the configuration as well as to the fine-structure splitting. The radial parts of the one-electron functions expressed in analytic forms as a sum of Slater-type orbitals, are given by equation (3). The wave functions given by equation (6) are used to calculate the excitation energies of the fine-structure levels, length and velocity forms of the oscillator strengths, and transition probabilities among the fine-structure levels.

The radiative lifetime of an excited state is calculated from our radiative transition probabilities (A_{ji}) using the relation [31]

$$\tau_j = 1/\Sigma_i A_{ji}, \tag{7}$$

where the sum over i is over all accessible final states and ΔE $(=E_j - E_i)$ is the transition energy.

3 Results and discussion

In Table 2 our calculated fine-structure excitation energies relative to the ground level are compared with the experimental levels compiled by Shirai et al. [26] and the multi-configuration Hartree-Fock (MCHF) calculations [30] of Tachiev and Froese-Fischer [18]. In general, our ab initio calculation, denoted "Present (a)", is in good agreement (better than 1.8%) with the corresponding experimental values [26]. In order to keep our ab initio energies as close as possible to the experimental values, we have made small J-dependent adjustments to the diagonal elements of the Hamiltonian matrices. These adjustments improve

Table 2. Fine structure energy levels (in cm^{-1}) of Cr XIII relative to the ground level.

				Present Cal.				
Key	Conf.	Term	J	(a)	(b)	Expt.	MCHF	Leading %
1	$3s^2$	$^1\mathrm{S}$	0	0	0	0	0	97.2, 2.4(10)
2	$3s3p$	$^3\mathrm{P}^\mathrm{o}$	0	202903	203520	203444	202644	99.5
3			1	206587	207465	207399	206667	99.1
4			2	214966	216627	216557	215833	99.5
5		$^1\mathrm{P}^\mathrm{o}$	1	307631	304679	304629	303478	96.8
6	$3p^2$	$^3\mathrm{P}$	0	484166	482189	482122	481728	97.7
7		$^1\mathrm{D}$	2	483269	482319	483144	482477	70.8, 20.7(14), 7.6(9)
8		$^3\mathrm{P}$	1	489592	488303	488223	488141	99.4
9			2	499359	499124	499174	499119	89.3, 10.0(7)
10		$^1\mathrm{S}$	0	572803	569699	569421	569111	93.4, 2.7(1)
11	$3s3d$	$^3\mathrm{D}$	1	590592	588658	588562	589784	99.7
12			2	591298	589247	589150	590201	99.7
13			3	592405	590159	590063	591297	99.7
14		$^1\mathrm{D}$	2	667501	663558	662428	662986	77.7, 18.8(7), 2.6(9)
15	$3p3d$	$^3\mathrm{F}^\mathrm{o}$	2	806905	805249	805156	805795	90.8, 8.4(18)
16			3	812722	811534	811454	812573	99.0
17			4	819449	818823	818730	820296	99.7
18		$^1\mathrm{D}^\mathrm{o}$	2	821730	820034	819961	820027	89.6, 8.6(15)
19		$^3\mathrm{P}^\mathrm{o}$	2	856183	853135	852734	853530	64.3, 33.5(24)
20		$^3\mathrm{D}^\mathrm{o}$	1	856587	853535	853150	854031	73.4, 25.8(23)
21		$^3\mathrm{P}^\mathrm{o}$	0	863223	859781	859662	862212	99.3
22		$^3\mathrm{D}^\mathrm{o}$	3	864108	861014	860904	861857	98.8
23		$^3\mathrm{P}^\mathrm{o}$	1	863848	861246	861427	862575	73.6, 25.4(20)
24		$^3\mathrm{D}^\mathrm{o}$	2	864518	861651	861799	862796	65.7, 33.4(19)
25		$^1\mathrm{F}^\mathrm{o}$	3	925279	920690	920560	922143	98.5
26		$^1\mathrm{P}^\mathrm{o}$	1	936884	931960	931754	933011	95.8, 2.7(5)
27	$3d^2$	$^3\mathrm{F}$	2	1191507	1187875	1187767	1190538	99.3
28			3	1192645	1188854	1188753	1191908	99.5
29			4	1194056	1190012	1189901	1192988	99.4
30		$^1\mathrm{D}$	2	1219926	1215389	1215243	1217496	91.0, 7.0(34)
31		$^1\mathrm{G}$	4	1222361	1218017	1217906	1221509	98.7
32		$^3\mathrm{P}$	0	1222930	1218573	1218447	1221259	99.0
33			1	1223363	1218878	1218751	1221952	99.0
34			2	1224316	1219674	1219532	1222330	92.0, 7.0(30)
35		$^1\mathrm{S}$	0	1294426	1294375	——	1291256	95.5, 2.3(10)
36	$3s4s$	$^3\mathrm{S}$	1	1384962	1385333	1385260	1386786	98.8
37		$^1\mathrm{S}$	0	1406428	1400304	1400000	1407567	96.6
38	$3s4p$	$^3\mathrm{P}^\mathrm{o}$	0	1487360	1487452	——	1487743	98.3
39			1	1487716	1487973	——	1488184	80.4, 17.9(41)
40			2	1491601	1491730	——	1493043	98.4
41		$^1\mathrm{P}^\mathrm{o}$	1	1492085	1492795	1492920	1493070	76.9, 17.3(39)
42	$3s4d$	$^3\mathrm{D}$	1	1616455	1616307	1616210	1617064	95.4, 2.5(55)
43			2	1616920	1616525	1616450	1617697	90.4, 5.3(45), 3.5(56)
44			3	1617679	1617233	1617160	1618503	96.1
45		$^1\mathrm{D}$	2	1618948	1617665	1617480	1619268	90.0, 5.4(43)
46	$3p4s$	$^3\mathrm{P}^\mathrm{o}$	0	1639356	1639447	1652000	1638727	98.3
47			1	1641933	1642027	——	1641305	91.8, 6.5(49)
48			2	1651493	1652094	——	1652277	98.4
49		$^1\mathrm{P}^\mathrm{o}$	1	1664285	1664407	——	1662940	87.3, 6.1(47)
50	$3s4f$	$^3\mathrm{F}^\mathrm{o}$	2	1679260	1678587	1678490	1680115	99.0
51			3	1679380	1678632	1678570	1680409	99.0
52			4	1679552	1678838	1678740	1680606	99.1
53		$^1\mathrm{F}^\mathrm{o}$	3	1692990	1690582	1690860	1692807	97.8
54	$3p4p$	$^1\mathrm{P}$	1	1726593	1726653	——	1724865	68.0, 23.4(55), 6.2(59)
55		$^3\mathrm{D}$	1	1736193	1736234	——	1735516	63.0, 27.8(54), 4.0(42), 4.0(59)
56			2	1738157	1738220	——	1737495	90.0, 4.5(60)

Table 2. *Continued.*

Key	Conf.	Term	J	Present Cal.		Expt.	MCHF	Leading %
				(a)	(b)			
57		^{3}P	0	1742917	1743000	——	1742690	96.6, 2.5(63)
58		^{3}D	3	1746845	1746104	1746000	1747591	95.6, 3.3(44)
59		^{3}P	1	1746966	1746951	——	1747377	79.6, 12.3(61), 6.9(55)
60			2	1752167	1752103	1752000	1753083	89.9, 5.6(62), 3.6(56)
61		^{3}S	1	1755338	1754289	1754000	1755483	83.9, 8.9(59), 3.2(55)
62		^{1}D	2	1767306	1767340	——	1767170	87.4, 4.3(60), 3.5(45)
63		^{1}S	0	1793551	1793524	——	1791422	92.9, 2.4(57)
64	$3p4d$	^{1}F$^{\rm o}$	3	1881134	1844573	1847000	1880489	90.5, 4.9(68)
65		^{1}D$^{\rm o}$	2	1862844	1863318	——	1861018	74.3, 21.2(69)
66		^{3}D$^{\rm o}$	2	1863502	1865484	1866000	1862139	74.0, 20.5(69)
67			1	1862517	1865804	1866000	1861301	90.8, 6.4(72)
68		^{3}F$^{\rm o}$	3	1875157	1868806	1870000	1874797	75.2, 19.9(70), 3.4(64)
69			2	1874055	1874568	——	1873543	57.0, 22.4(65), 19.0(66)
70		^{3}D$^{\rm o}$	3	1864637	1876451	1871000	1863271	78.5, 18.3(68)
71		^{3}F$^{\rm o}$	4	1880325	1880411	——	1880705	98.6
72		^{3}P$^{\rm o}$	1	1887013	1887301	——	1885375	76.0,19.4(75), 3.0(67)
73			0	1889483	1889573	——	1888588	98.6
74			2	1885851	1890774	1891000	1884377	92.9, 3.5(66)
75		^{1}P$^{\rm o}$	1	1893076	1893212	——	1890528	75.4, 15.6(72), 4.5(67)
76	$3p4f$	^{3}G	3	1922506	1913033	1916020	1917014	64.9, 28.1(79), 6.4(77)
77		^{3}F	3	1930360	1917013	1920670	1931246	51.6, 25.8(76), 18.7(79), 3.4(83)
78		^{3}G	4	1923277	1921045	1920470	1922722	68.4, 29.2(82)
79		^{1}F	3	1917788	1925030	——	1922312	52.4, 35.0(77), 8.5(76), 3.8(83)
80		^{3}F	2	1925233	1925249	——	1925589	92.6, 5.7(84)
81		^{3}G	5	1932432	1930076	1929970	1933068	99.4
82		^{3}F	4	1932354	1930842	1931340	1933534	70.3, 27.8(78)
83		^{3}D	3	1943636	1940597	1940700	1943793	90.9, 6.6(77)
84			2	1946001	1944630	1944400	1946215	91.0, 4.8(80)
85			1	1948213	1946626	1946500	1948657	97.8
86		^{1}G	4	1959336	1953284	1953000	1955862	85.3, 3.0(78)
87		^{1}D	2	1963636	1963668	——	1961012	95.0, 2.0(80)

Present (a): ab initio calculation; Present (b): Adjusted energy calculation. Expt: Shirai et al. [26]. MCHF: Calculation of Tachiev and Froese Fischer [18].

the accuracy of the mixing coefficients b_{ij} in equation (6), which depends in part on the accuracy of the eigenvalues. This is a justifiable fine-tuning technique [32] and is particularly useful for the calculation of intercombination lines [33]. These adjustments also affect the composition of the eigenvectors slightly. In a way, they correct the ab initio approach for the neglected core-valence correlation, which has been shown to contribute significantly in neutral magnesium (see, for instance: Jönsson et al. [34]). Our adjusted theoretical energies, "Present (b)", are also listed in Table 2 and are now in excellent agreement (better than 0.5%) with the experiment [26]. The ordering of our calculated levels (Present (b)) are the same as that of the experiment [26] except for the levels 77 and 78. It may be mentioned that these two levels are very close in their energy values. We have arranged our adjusted energy levels in ascending order. In general, the calculated levels of Tachiev and Froese-Fischer [18] are closer to our ab initio energies (Present (a)).

The last column in Table 2 represents the leading percentage composition of the various levels (corresponding to Present (b)). The first number of each entry in this column represents the leading percentage of the level corresponding to the level number under the first column followed by a set of numbers of the form $M(N)$. These mean that the next leading percentage is M% of the level number N in the first column and so on. As can be seen, the mixing among several fine-structure levels (7 & 14, 19 & 24, 20 & 23, 54 & 55, 66 & 69, 76 & 77, 78 & 82, 77 & 79) is found to be very strong. These levels are identified by their dominant eigenvector [35].

In Table 3, we have tabulated our calculated wavelengths, oscillator strengths in both the length f_L and velocity f_V forms and transition probabilities in the length form A_L for only those transitions for which experimental/theoretical results are available to compare with our calculations. In calculating these parameters, we used our adjusted theoretical energy splittings, corresponding to the Present (b) in Table 2. The keys of lower and upper levels involved in a transition are given in Table 2. For all strong and even for some relatively weaker transitions, a good agreement between the length (f_L) and velocity (f_V) values of the oscillator strengths indicates to some extent the accuracy of the wave functions used in our CIV3

Table 3. Comparison of wavelengths (in Å), oscillator strengths for some transitions of Cr XIII.

		Present calculation				Experiment		Other calculations	
Trans.		λ	f_L	f_V	A_L	λ	f	λ	f
1	3	482.01	1.826E-03	4.200E-03	1.748E+07	482.17	1.90E-03	483.87^a	2.17E-03^a, 1.70E-03^b, 2.04E-03^c
1	5	328.21	8.792E-01	8.888E-01	1.815E+10	328.27	9.02E-01	329.51^a	8.43E-01^a, 8.37E-01^b, 9.01E-01^c
1	20	117.16	4.366E-08	3.102E-06	7.072E+03	——	——	117.09^a	2.38E-07^a
1	23	116.11	3.264E-07	3.980E-09	5.383E+04	——	——	115.93^a	1.65E-07^a
1	26	107.30	1.186E-03	1.352E-03	2.291E+08	——	——	107.18^a	1.30E-03^a
1	39	67.21	6.616E-02	6.381E-02	3.257E+10	——	——	67.20^a	1.14E-01^a
1	41	66.99	2.803E-01	2.806E-01	1.389E+11	66.98	3.38E-01	66.98^a	2.64E-01^a
1	47	60.90	5.022E-04	5.421E-04	3.011E+08	——	——	60.93^a	4.64E-04^a
1	49	60.08	4.667E-03	5.313E-03	2.874E+09	——	——	60.13^a	2.70E-03^a
1	67	53.60	1.134E-04	1.440E-04	8.779E+07	——	——	53.73^a	3.71E-04^a
1	72	52.99	3.447E-04	3.986E-04	2.730E+08	——	——	53.04^a	2.14E-03^a
1	75	52.82	1.641E-03	1.783E-03	1.308E+09	——	——	52.90^a	4.28E-03^a
2	8	351.14	3.087E-01	3.032E-01	5.567E+09	351.15	3.10E-01	350.27^a	2.96E-01^a
2	11	259.65	3.509E-01	3.418E-01	1.157E+10	259.66	3.50E-01	258.31^a	3.42E-01^a
2	33	98.49	9.733E-05	1.024E-04	2.231E+07	——	——	98.11^a	1.30E-04^a
2	36	84.62	7.158E-02	7.570E-02	2.223E+10	——	——	84.45^a	7.75E-02^a
2	42	70.78	2.892E-01	3.017E-01	1.284E+11	——	——	70.70^a	3.03E-01^a
2	54	65.65	7.059E-03	6.147E-03	3.641E+09	——	——	65.69^a	1.07E-02^a
3	6	364.00	9.869E-02	1.032E-01	1.491E+10	364	1.00E-01	363.56^a	9.43E-02^a
3	7	363.83	1.801E-02	1.666E-02	5.446E+08	362.66	2.10E-02	362.57^a	2.32E-02^a
3	8	356.08	7.585E-02	7.626E-02	3.990E+09	356.1	7.67E-02	355.27^a	7.28E-02^a
3	9	342.87	1.134E-01	1.088E-01	3.861E+09	342.73	1.00E-01	341.94^a	1.03E-01^a
3	10	276.06	5.212E-04	4.136E-04	1.368E+08	——	——	275.06^a	6.47E-04^a
3	11	262.33	8.661E-02	8.580E-02	8.394E+09	262.36	8.67E-02	261.02^a	8.41E-02^a
3	12	261.93	2.605E-01	2.586E-01	1.520E+10	261.95	2.60E-01	260.73^a	2.54E-01^a
3	14	219.25	1.777E-03	1.171E-03	1.479E+08	——	——	219.15^a	2.35E-03^a
3	27	102.00	3.611E-08	1.086E-10	1.389E+04	——	——	101.64^a	5.11E-08^a
3	30	99.21	1.860E-05	1.494E-05	7.560E+06	——	——	98.93^a	2.12E-05^a
3	32	98.90	2.508E-05	3.079E-05	5.131E+07	——	——	98.56^a	3.49E-05^a
3	33	98.87	2.295E-05	2.481E-05	1.566E+07	——	——	98.49^a	3.06E-05^a
3	34	98.79	3.144E-05	3.311E-05	1.289E+07	——	——	98.46^a	4.40E-05^a
3	35	92.00	1.571E-06	3.704E-06	3.714E+06	——	——	92.2^a	2.93E-06^a
3	36	84.90	7.261E-02	7.554E-02	6.719E+10	——	——	84.74^a	7.83E-02^a
3	37	83.83	8.726E-05	1.656E-04	2.485E+08	——	——	83.27^a	1.43E-04^a
3	42	70.98	7.292E-02	7.526E-02	9.654E+10	——	——	70.9^a	7.64E-02^a
3	43	70.97	2.087E-01	2.169E-01	1.658E+11	——	——	70.87^a	2.24E-01^a
3	45	70.91	8.410E-03	8.061E-03	6.694E+09	——	——	70.79^a	2.61E-03^a
3	54	65.82	9.122E-03	8.434E-03	1.404E+10	——	——	65.87^a	1.17E-02^a
4	7	376.38	2.183E-02	2.434E-02	1.028E+09	375.11	2.60E-02	375.03^a	2.81E-02^a
4	8	368.09	7.313E-02	7.853E-02	6.001E+09	368.1	7.40E-02	367.23^a	7.00E-02^a
4	9	353.99	2.057E-01	2.054E-01	1.095E+10	353.84	1.90E-01	353.0^a	1.90E-01^a
4	11	268.79	3.396E-03	3.508E-03	5.226E+08	268.81	3.40E-03	267.42^a	3.28E-03^a
4	12	268.37	5.118E-02	5.294E-02	4.740E+09	268.38	5.20E-02	267.12^a	4.96E-02^a
4	13	267.72	2.864E-01	2.973E-01	1.904E+10	267.74	2.86E-01	266.34^a	2.79E-01^a
4	14	223.75	4.272E-05	1.436E-05	5.691E+06	——	——	223.64^a	5.68E-05^a
4	27	102.96	9.635E-09	1.193E-09	6.063E+03	——	——	102.6^a	1.21E-08^a
4	28	102.86	9.888E-08	6.384E-09	4.453E+04	——	——	102.45^a	1.14E-07^a
4	30	100.12	1.683E-06	3.571E-06	1.120E+06	——	——	99.83^a	9.24E-07^a
4	33	99.78	1.446E-05	2.050E-05	1.615E+07	——	——	99.39^a	2.13E-05^a
4	34	99.70	5.850E-05	6.578E-05	3.926E+07	——	——	99.35^a	8.13E-05^a
4	36	85.56	7.572E-02	7.598E-02	1.150E+11	——	——	85.4^a	8.11E-02^a

Table 3. *Continued.*

Trans.		Present calculation				Experiment		Other calculations	
		λ	f_L	f_V	A_L	λ	f	λ	f
4	42	71.44	2.990E-03	3.019E-03	6.511E+09	——	——	71.37[a]	3.12E-03[a]
4	43	71.43	4.217E-02	4.266E-02	5.512E+10	——	——	71.33[a]	4.54E-02[a]
4	44	71.40	2.470E-01	2.510E-01	2.308E+11	——	——	71.29[a]	2.56E-01[a]
4	45	71.38	2.360E-03	2.416E-03	3.090E+09	——	——	71.25[a]	9.86E-04[a]
4	54	66.22	4.449E-06	2.592E-06	1.128E+07	——	——	66.27[a]	3.70E-06[a]
4	55	65.81	1.321E-04	9.812E-05	3.391E+08	——	——	65.8[a]	2.03E-04[a]
4	56	65.72	1.991E-03	1.747E-03	3.075E+09	——	——	65.72[a]	2.62E-03[a]
5	7	562.93	1.013E-01	9.469E-02	1.279E+09	560.18	1.00E-01	——	——-
5	10	377.33	1.160E-01	1.135E-01	1.630E+10	377.65	1.10E-01	——	——-
5	14	278.65	7.103E-01	7.170E-01	3.662E+10	279.48	7.00E-01	——	——-
7	18	296.11	1.856E-01	1.854E-01	1.412E+10	296.89	1.70E-01	——	——-
7	25	228.12	2.171E-01	2.298E-01	1.988E+10	228.62	2.00E-01	——	——-
7	26	222.40	1.881E-03	1.760E-03	4.227E+08	222.91	1.30E-03	——	——-
9	22	276.33	3.752E-01	3.904E-01	2.341E+10	276.44	3.60E-01	——	——-
10	26	276.04	7.553E-01	7.749E-01	2.204E+10	276	7.30E-01	——	——-
11	15	461.70	1.447E-01	1.410E-01	2.717E+09	461.69	1.50E-01	——	——-
12	15	462.96	2.134E-02	2.216E-02	6.642E+08	462.95	2.20E-02	——	——-
12	16	449.87	1.428E-01	1.326E-01	3.363E+09	449.83	1.50E-01	——	——-
12	22	367.96	3.522E-02	3.351E-02	1.239E+09	367.98	3.80E-02	——	——-
13	15	464.92	3.188E-04	3.130E-04	1.378E+07	464.92	2.86E-04	——	——-
13	16	451.72	1.958E-02	2.013E-02	6.400E+08	451.69	2.14E-02	——	——-
13	17	437.32	1.615E-01	1.445E-01	4.381E+09	437.32	1.71E-01	——	——-
13	22	369.20	1.305E-01	1.349E-01	6.383E+09	369.22	1.30E-01	——	——-
14	18	639.08	3.406E-02	3.220E-02	5.562E+08	634.78	3.60E-02	——	——-
14	25	388.91	4.370E-01	4.211E-01	1.377E+10	387.4	4.60E-01	——	——-
14	26	372.58	1.243E-01	1.347E-01	9.955E+09	371.3	1.30E-01	——	——-
25	31	336.33	4.032E-01	3.762E-01	1.849E+10	336.31	4.09E-01	——	——-

Expt.: Shirai et al. [26]; [a] calculation of Tachiev and Froese Fischer [18]; [b] calculation of Safronova et al. [16]; [c] calculation of Huang and Johnson [36].

calculation. The magnitudes of the oscillator strengths for most intercombination transitions are smaller by several orders of magnitude than those for allowed transitions and there is a significant difference between the f_L and f_V values for several of these transitions. In such cases the length value of our oscillator strength is recommended since it remains stable with respect to the addition of more and more configurations. It may be mentioned that the small oscillator strengths are sensitive to cancellation effects.

For most of the strong transitions, our results for wavelengths (λ) and the oscillator strengths (f_L) are in reasonably good agreement with the experimental values [26] as well as the theoretical results [18]. However, for a few relatively weaker transitions, the calculated values of Tachiev and Froese-Fischer [18] show considerable difference with our calculation. For the transitions $3s^2(^1\mathrm{S}_0)$–$3s3p(^1\mathrm{P}_1, {}^3\mathrm{P}_1)$ our results for f_L also show reasonable good agreement with the theoretical results of Safronova et al. [16] and Huang and Johnson [36].

In Table 4 we reported our calculated lifetimes (in seconds) for all fine-structure levels. These are compared with the available experimental values of Curtis [37] and the other theoretical results of Safronova et al. [16], and Tachiev and Froese-Fischer [18]. For the longer-lived level $3s3p(^3\mathrm{P}_1)$, our calculated value is found to be in excellent agreement with the experimental result of Curtis [37] compared to other theoretical calculations [16,18]. Also, for $3s3p(^1\mathrm{P}_1)$ level, our lifetime is in better agreement with the experiment [37] compared to theoretical results of Safronova et al. [16], and Tachiev and Froese-Fischer [18]. In general, our calculated lifetimes are in reasonable good agreement (10–15%) with the other theoretical values [16,18] for most levels. However, for the levels $3p4d(^{1,3}\mathrm{D}_2, {}^{1,3}\mathrm{F}_3)$, a very significant difference ($25-50\%$) between our calculated lifetimes and the theoretical results of Tachiev and Froese-Fischer [18] is noticed.

4 Conclusions

In conclusion, we have presented our calculated excitation energies for the lowest 86 fine-structure levels from ground state of Cr XIII as well as oscillator strengths and radiative decay rates for the transitions among the fine-structure levels of the terms belonging to the $(1s^2 2s^2 2p^6)3s^2$, $3s3p$, $3s3d$, $3s4s$, $3s4p$, $3s4d$, $3s4f$, $3p^2$, $3p3d$, $3p4s$, $3p4p$, $3p4d$, $3p4f$ and $3d^2$ configurations of Cr XIII. In this calculation, we have used an extensive set of CI wave functions and included correlation effects in the excitation up to the $5g$ orbital. Our calculated excitation energies, including their ordering, are in excellent

Table 4. Lifetimes (in second) of fine-structure levels in Cr XIII.

Conf.	Term	J	Present	Expt.	MCHF	MBPT
$3s3p$	$^3\mathrm{P}^o$	1	5.721E-08	5.47E-08	4.864E-08	6.13E-08
$3s3p$	$^1\mathrm{P}^o$	1	5.510E-11	5.32E-11	5.794E-11	5.78E-11
$3p^2$	$^3\mathrm{P}$	0	6.693E-11	——	6.986E-11	6.44E-11
	$^1\mathrm{D}$	2	3.508E-10	——	3.027E-10	3.48E-10
	$^3\mathrm{P}$	1	6.426E-11	——	6.671E-11	6.71E-11
		2	6.654E-11	——	7.146E-11	6.84E-11
	$^1\mathrm{S}$	0	6.083E-11	——	6.396E-11	6.98E-11
$3s3d$	$^3\mathrm{D}$	1	4.878E-11	——	4.961E-11	5.10E-11
		2	5.013E-11	——	5.108E-11	5.26E-11
		3	5.252E-11	——	5.340E-11	5.49E-11
	$^1\mathrm{D}$	2	2.720E-11	——	2.865E-11	2.96E-11
$3p3d$	$^3\mathrm{F}^o$	2	2.105E-10	——	2.080E-10	2.15E-10
		3	2.425E-10	——	2.502E-10	2.55E-10
		4	2.283E-10	——	2.367E-10	2.39E-10
	$^1\mathrm{D}^o$	2	6.150E-11	——	6.707E-11	6.50E-11
	$^3\mathrm{P}^o$	2	3.634E-11	——	3.706E-11	3.71E-11
	$^3\mathrm{D}^o$	1	3.028E-11	——	3.158E-11	3.62E-11
	$^3\mathrm{P}^o$	0	3.876E-11	——	3.974E-11	3.97E-11
	$^3\mathrm{D}^o$	3	2.869E-11	——	2.960E-11	2.99E-11
	$^3\mathrm{P}^o$	1	3.518E-11	——	3.601E-11	3.18E-11
	$^3\mathrm{D}^o$	2	3.116E-11	——	3.283E-11	3.32E-11
	$^1\mathrm{F}^o$	3	2.736E-11	——	2.715E-11	2.96E-11
	$^1\mathrm{P}^o$	1	3.039E-11	——	3.142E-11	3.25E-11
$3d^2$	$^3\mathrm{F}$	2	2.986E-11	——	3.040E-11	2.33E-11
		3	3.075E-11	——	3.117E-11	3.17E-11
		4	3.174E-11	——	3.234E-11	3.28E-11
	$^1\mathrm{D}$	2	2.564E-11	——	2.616E-11	2.37E-11
	$^1\mathrm{G}$	4	5.376E-11	——	5.397E-11	5.59E-11
	$^3\mathrm{P}$	0	2.386E-11	——	2.423E-11	2.43E-11
		1	2.399E-11	——	2.438E-11	2.83E-11
		2	2.466E-11	——	2.509E-11	2.25E-11
	$^1\mathrm{S}$	0	1.888E-11	——	1.992E-11	2.04E-11
$3s4s$	$^3\mathrm{S}$	1	4.885E-12	——	4.527E-12	——
	$^1\mathrm{S}$	0	7.740E-12	——	7.236E-12	——
$3s4p$	$^3\mathrm{P}^o$	0	2.207E-11	——	2.157E-11	——
		1	1.263E-11	——	9.601E-12	——
		2	2.232E-11	——	2.193E-11	——
	$^1\mathrm{P}^o$	1	5.258E-12	——	5.507E-12	——
$3s4d$	$^3\mathrm{D}$	1	4.215E-12	——	4.016E-12	——
		2	4.347E-12	——	4.095E-12	——
		3	4.240E-12	——	4.085E-12	——
	$^1\mathrm{D}$	2	6.947E-12	——	7.189E-12	——
$3p4s$	$^3\mathrm{P}^o$	0	7.252E-12	——	6.935E-12	——
		1	7.050E-12	——	6.632E-12	——
		2	7.296E-12	——	6.899E-12	——
	$^1\mathrm{P}^o$	1	4.929E-12	——	4.721E-12	——
$3s4f$	$^3\mathrm{F}^o$	2	1.948E-12	——	2.027E-12	——
		3	1.949E-12	——	2.025E-12	——
		4	1.946E-12	——	2.025E-12	——
	$^1\mathrm{F}^o$	3	2.003E-12	——	2.087E-12	——
$3p4p$	$^1\mathrm{P}$	1	7.283E-12	——	6.925E-12	——
	$^3\mathrm{D}$	1	8.460E-12	——	7.804E-12	——
		2	9.302E-12	——	8.593E-12	——
	$^3\mathrm{P}$	0	7.669E-12	——	7.200E-12	——
	$^3\mathrm{D}$	3	9.320E-12	——	8.505E-12	——
	$^3\mathrm{P}$	1	7.659E-12	——	7.210E-12	——
		2	7.644E-12	——	7.164E-12	——
	$^3\mathrm{S}$	1	7.293E-12	——	6.823E-12	——
	$^1\mathrm{D}$	2	6.094E-12	——	6.150E-12	——
	$^1\mathrm{S}$	0	8.410E-12	——	8.356E-12	——
$3p4d$	$^1\mathrm{F}^o$	3	3.118E-12	——	4.034E-12	——
	$^1\mathrm{D}^o$	2	1.131E-11	——	7.771E-12	——
	$^3\mathrm{D}^o$	2	4.328E-12	——	5.051E-12	——
		1	3.536E-12	——	3.514E-12	——
	$^3\mathrm{F}^o$	3	1.164E-11	——	5.387E-12	——
		2	1.081E-11	——	1.180E-11	——
	$^3\mathrm{D}^o$	3	4.180E-12	——	4.171E-12	——
	$^3\mathrm{F}^o$	4	5.461E-11	——	5.927E-11	——
	$^3\mathrm{P}^o$	1	5.710E-12	——	5.278E-12	——
		0	6.506E-12	——	6.451E-12	——
		2	6.154E-12	——	6.172E-12	——
	$^1\mathrm{P}^o$	1	4.542E-12	——	4.873E-12	——
$3p4f$	$^3\mathrm{G}$	3	1.897E-12	——	1.932E-12	——
	$^3\mathrm{F}$	3	1.955E-12	——	1.996E-12	——
	$^3\mathrm{G}$	4	1.885E-12	——	1.973E-12	——
	$^1\mathrm{F}$	3	1.891E-12	——	1.985E-12	——
	$^3\mathrm{F}$	2	1.976E-12	——	2.068E-12	——
	$^3\mathrm{G}$	5	1.827E-12	——	1.906E-12	——
	$^3\mathrm{F}$	4	1.938E-12	——	2.015E-12	——
	$^3\mathrm{D}$	3	1.830E-12	——	1.921E-12	——
		2	1.817E-12	——	1.915E-12	——
		1	1.795E-12	——	1.890E-12	——
	$^1\mathrm{G}$	4	2.318E-12	——	2.431E-12	——
	$^1\mathrm{D}$	2	2.102E-12	——	2.170E-12	——

Expt: curtis [37]. MCHF: calculation of Tachiev and Froese Fischer [18]; MBPT: calculation of Safronova et al. [16]

agreement (better than 0.5%) with the available experimental results. Also, our calculated wavelengths, absorption oscillator strengths, for most transitions, are in good agreement with the available experimental and the other theoretical results. However, for relatively weaker transitions the calculations of Tachiev and Froese-Fischer [18] show considerable difference with our results. For the $3s3p(^{1,3}\mathrm{P}_1)$ levels, our calculated lifetimes are found to be in better agreement with the experimental result of Curtis [37] compared to other theoretical calculations [16, 18]. However, for few fine-structure levels, a very significant difference between our calculated lifetimes and the theoretical results of Tachiev and Froese-Fischer [18] is noticed. These differences/variations in the calculated lifetimes call for further careful experimental and theoretical investigations. Finally, we believe that the present results are the most extensive and definitive to date and should be useful in many astrophysical applications and in technical plasma modeling.

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