

Fine-structure energy levels, oscillator strengths and lifetimes of chlorine-like chromium

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Abstract. We have done relativistic calculations for the evaluation of energy levels, oscillator strengths, transition probabilities and lifetimes for Cr VIII ion. Use has been made of configuration interaction technique by including Briet–Pauli approximation. The energies of various levels from the ground state to excited levels of $3s3p^6$, $3s^23p^43d$, $3s^23p^44s$, $3s^23p^44d$ of Cr VIII are given in LSJ coupling scheme after fine-tuning and are compared with the experimental results compiled in the NIST Data Base. Many new lines have been predicted which have not appeared so far in the NIST Data.

Keywords. Relativistic fine-structure levels; oscillator strengths; lifetimes.

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1. Introduction

Hot fusion plasmas, e.g. in pinches, tokamaks and stellartors, which nominally consists of hydrogen isotopes, are contaminated by impurity atoms of light and heavier atoms. Cr ions are one important impurities of hot fusion plasmas. Besides their nuisance values they are also useful as diagnostic tools for finding the temperature and density of hot plasmas [1]. Further, the energies and transition rates of these ions have been used for the determination of radiative opacities of stellar envelopes [2], for spectral diagnostics of solar, stellar and laboratory plasmas and for plasma modeling. Also, the excitation energies and oscillator strengths in highly stripped ions are needed for estimating the energy losses through impurity ions in plasmas.

Some theoretical calculations of level energies and oscillator strengths for transitions in Cr VIII have been reported. Among these, Fawcett [3] has reported level energies and oscillator strengths for some of the transitions from $3s^23p^5$ to $3s3p^6$, $3s^23p^43d$ and $3s^23p^44s$ using MCDF method. Recently, Berrington *et al* [4] have calculated oscillator strengths and lifetimes using the Briet–Pauli R-Matrix method for $3s^23p^5\ ^2P_{3/2,1/2}^o$ to $3s3p^6\ ^2S_{1/2}^e$ transition in Cl-like ions including Cr VIII. Biémont and Träbert [5] performed Hartree–Fock calculations with relativistic

corrections on Cl-like ions from Ar II to Ge XVII for the same transitions considered by Berrington *et al*.

As accurate atomic data are needed for the interpretation of spectra observed by space mission in terms of physical conditions in the astrophysical sources [6] and because of the importance of the Cl-like ions in astrophysics, plasma physics and spectroscopy, in the present work, we have calculated level energies, oscillator strengths for the transitions from the ground state $3s^23p^5\ ^2P_{3/2,1/2}^o$ to those of $3s3p^6$ and $3s^23p^4\ nl$ ($nl = 3d, 4s, 4d$) of Cr VIII in LSJ coupling. The energies of the various levels are fine-tuned with respect to the experimental results by making small adjustments to the diagonal elements of the Hamiltonian matrices [7]. Using accurate energy separations, we have also calculated the transition probabilities and lifetimes of excited levels. The relativistic effects are included in the Briet–Pauli approximation via one-body mass correction, Darwin and spin–orbit interaction terms in the non-relativistic Hamiltonian [8]. A point worth mentioning is that we have predicted many new lines, which are yet to be observed.

2. Method of calculation

The wave functions describing the atomic states included in these calculations were obtained using configuration interaction code CIV3 [9,10].

The configuration interaction wave functions are represented as

$$\Psi(\text{LSJ}) = \sum_{i=1}^M a_i \Phi_i(\alpha_i \text{LSJ}), \quad (1)$$

where $\{\Phi_i\}$ are single-configuration wave functions whose angular momenta are coupled to form a total $L_i S_i J$ in intermediate coupling. The radial part of each orbital is expressed in analytic form as

$$P_{nl}(r) = \sum_{j=1}^k C_{jnl} \frac{(\zeta_{jnl})^{I_{jnl}+1/2}}{[(2I_{jnl})!]^{1/2}} r^{I_{jnl}} \exp(-\zeta_{jnl}r) \quad (2)$$

and are chosen to satisfy the orthonormality conditions

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) dr = \delta_{nn'}, \quad l < n' \leq n. \quad (3)$$

If we form the Hamiltonian matrix whose typical element is $\langle \Phi_i H \Phi_j \rangle$ then the eigenvalues form upper bounds to the energies of the states with a particular symmetry with $(\text{LSJ}\pi)$ and corresponding eigenvectors give the CI coefficients $\{a_i\}$ in (1). This upper bound property of the eigenvalues provides a set of variational principles to enable us to optimize the radial parameter in (2).

The wave functions for all ionic states have been constructed in the form (1) from a common set of radial functions and we have used non-relativistic Hamiltonian for the optimization of orbitals. Fourteen orthogonal one-electron orbitals are used in our calculations. The process of optimizing the radial functions is given in table 1.

Table 1. Method of determining the radial functions.

Orbital	Process of optimization	
1s, 2s, 2p, 3s	Hartree–Fock orbitals of $3p^4(^1D)$ of sulphur-like chromium (Cr IX) [11]	
3p	Exponents taken from the Hartree–Fock orbital of $3p^4(^1D)$ of Cr IX; Coefficient reoptimized on $3p^44s(^4P^e)$ of Cr VIII	
	Eigenvalue minimized	Configurations
3d	$3s3p^6\ ^2S^e$	$3s^23p^43d$
4s	$3s^23p^44s\ ^4P^e$	$3s^23p^44s$
4p	$3s^23p^44p\ ^4D^o$	$3s^23p^44p$
4d	$3p^43d\ ^2D^e$	$3p^43d, 3p^44d$
4f	$3p^43d\ ^4P^e$	$3p^43d, 3p^44d, 3p^44s, 3p^33d4f$
5s	$3p^44p\ ^4D^o$	$3p^44p, 3p^34s5s$
5p	$3p^44p\ ^4P^o$	$3p^44p, 3p^45p$
5d	$3p^44d\ ^2D^e$	$3p^43d, 3p^44d, 3p^45d$
5f	$3p^44p\ ^4D^o$	$3p^44p, 3p^44f, 3p^45f$

We have used Hartree–Fock functions for 1s, 2s, 2p and 3s orbitals of $3p^4(^3P)$ of Cr IX [11]. The coefficients of 3p orbital are reoptimized on $3p^44s(^4P)$ of Cr VIII by taking the exponents from the Hartree–Fock orbitals of $3p^4(^3P)$ of Cr IX. The 3d orbital is chosen to give an accurate representation of $3s3p^6$ – $3s^23p^43d$ correlation effects in the lowest 2S state. The 4d orbital is optimized on $3p^43d\ ^2D^e$ state with $3p^43d$ and $3p^44d$ configurations so that the spectroscopic 3d orbital is a linear combination of 3d and 4d orbitals. All other orbitals listed in table 1 are optimized to give the best overall representation of energies of the states.

The optimized parameters of the radial functions are shown in table 2. The CI wave functions include all possible angular momenta couplings of the configurations listed in table 3.

Table 2.

Parameters of the optimized orbitals of Cr VIII			
Orbitals	Expansion coefficients (C_i)	Power of r (p_i)	Exponents (ξ_i)
3p	–0.34964	2	10.12410
	–0.02716	2	17.46250
	0.63199	3	4.83287
	0.49919	3	3.92890
	–0.11496	3	8.52301

Table 2. *Continued.*

Parameters of the optimized orbitals of Cr VIII			
Orbitals	Expansion coefficients (C_I)	Power of r (p_i)	Exponents (ξ_I)
3d	0.96482	3	4.13049
	0.04966	3	7.90887
4s	0.07804	1	19.91316
	-0.86490	2	5.32686
	1.35153	3	5.29862
	-1.16957	4	2.61984
4p	0.20729	2	10.15934
	-0.77716	3	4.01324
	1.28319	4	2.55381
4d	0.44095	3	4.66502
	-1.05762	4	2.09454
4f	1.00000	4	4.61302
5s	1.05774	1	5.07789
	-6.45006	2	4.80498
	13.38916	3	4.72064
	-9.46133	4	4.73102
	1.56403	5	3.21702
5p	4.78722	2	17.24795
	-9.06115	3	16.94558
	6.29493	4	16.72604
	-1.53279	5	16.52049
5d	4.78692	3	7.22639
	-7.81251	4	7.05698
	3.59760	5	7.14088
5f	1.07342	4	4.29832
	-1.53315	5	3.29424

3. Result and discussion

The excitation energies of the fine-structure levels relative to the ground state are given in table 4, which are compared with the experimental values compiled in the NIST Data Base [12]. The disagreement between the present calculations and experimental results [12] is within 2%. In our calculations we have made small adjustments to the diagonal elements of the Hamiltonian matrices for bringing down the level energies closer to the experimental data. This process is called fine-tuning [7] and this is important to calculate accurate oscillator strengths and transition probabilities.

Table 3. Configuration used.

Odd parity $[1s^2 2s^2 2p^6] 3s^2 3p^5, 3s 3p^5 3d, 3p^5 3d^2, 3s^2 3p^3 4d^2, 3s^2 3p^4 4p, 3p^6 4p,$
 $3s 3p^5 4s, 3s 3p^5 4d, 3p^5 4s^2, 3p^5 4p^2, 3p^5 4d^2, 3s^2 3p^3 4s^2, 3s^2 3p^3 4d 4d, 3s^2 3p^4 4f,$
 $3s^2 3p^4 5f, 3s^2 3p^4 5p, 3s^2 3p^3 4s 5s, 3s 3p^5 5d, 3s^2 3p^3 3d^2, 3s^2 3p^3 5d^2, 3p^6 5p,$
 $3s^2 3p^3 4p^2, 3s^2 3p^3 4p 5p, 3s 3p^5 5s, 3s^2 3p^3 4s 4d, 3s^2 3p^3 4s 5d, 3s^2 3p^3 5s 5d,$
 $3s^2 3p^3 3d 5d, 3s^2 3p^3 4d 5d, 3p^6 4f, 3p^6 5f$

Even parity $[1s^2 2s^2 2p^6] 3s 3p^6, 3s^2 3p^4 3d, 3p^6 3d, 3s 3p^4 3d^2, 3s^2 3p^2 3d^3,$
 $3s^2 3p^4 4s, 3p^6 4s, 3s^2 3p^4 4d, 3p^6 4d, 3s 3p^5 4d, 3p^5 4s 4p, 3s 3p^4 3d 4s, 3p^4 3d^2 4d,$
 $3s^2 3p^4 5d, 3s^2 3p^4 5s, 3s^2 3p^3 3d 4p, 3s^2 3p^3 3d 4f, 3s^2 3p^3 4s 4p, 3s^2 3p^3 4s 4f,$
 $3s^2 3p^3 4d 4f, 3s^2 3p^3 4p 5s, 3s 3p^5 4f$

Table 4. Comparison of level energies for the transitions $3s^2 3p^5 \ ^2P_{3/2}^o \rightarrow$ levels (listed in the table) against an experimental value compiled in the NIST Atomic Spectra Database Levels Data. Other calculations: Fawcett (1987). Note: the label 3d refers to $3p^4(^3P)3d$; 3d' to $3p^4(^1D)3d$; 3d'' to $3p^4(^1S)3d$; 4d to $3p^4(^3P)4d$; 4d' to $3p^4(^1D)4d$; 4d'' to $3p^4(^1S)4d$; 4s to $3p^4(^3P)4s$; 4s' to $3p^4(^1D)4s$; 4s'' to $3p^4(^1S)4s$.

Level	Term	J	Energies (a.u.)			
			Cal.	Expt.	Fawcett	
$3s^2 3p^5$	$^2P^o$	3/2	0.00000	0.00000		
		1/2	0.04652	0.04507		
$3s 3p^6$	2S	1/2	1.08282	1.10293	1.10292	
		3d	4D	7/2	1.49908	
			5/2	1.49913		
			3/2	1.50205		
			1/2	1.50592		
3d'	2P	3/2	1.62946		1.65613	
		1/2	1.62955			
3d	4F	9/2	1.62630			
		7/2	1.64049			
		5/2	1.65060			
		3/2	1.65543			
3d'	2D	3/2	1.67067			
		5/2	1.69608			
3d	4P	1/2	1.68970			
		3/2	1.70109			
		5/2	1.71476			
3d	2F	7/2	1.72267			
		5/2	1.76137			
3d'	2G	9/2	1.75470			
		7/2	1.75480			
3d'	2F	5/2	1.88471			
		7/2	1.89642			

Table 4. Continued.

Level	Term	J	Energies (a.u.)		
			Cal.	Expt.	Fawcett
3d''	² D	3/2	2.00148		
		5/2	2.01409		
3d'	² S	1/2	2.12306	2.10290	2.10290
3d	² P	3/2	2.20955	2.18385	2.18336
		1/2	2.25637	2.20030	2.19952
3d	² D	5/2	2.24526	2.22245	2.22347
		3/2	2.28424	2.26070	2.26086
4s	⁴ P	5/2	3.35494	3.35290	
		3/2	3.37860	3.37650	3.37937
		1/2	3.46179		
4s	² P	3/2	3.41784	3.41560	3.41403
		1/2	3.44465	3.44340	3.44030
4s'	² D	5/2	3.50913	3.50490	3.50312
		3/2	3.51056	3.50630	
4s''	² S	1/2	3.67731	3.66900	3.67050
3p ⁶ 3d	² D	3/2	4.20163		
		5/2	4.20952		
4d	² D	5/2	4.32566	4.31100	
		3/2	4.32845	4.31600	
		1/2	4.39222	4.40300	
4s'	² S	1/2	4.39222	4.40300	
		3/2	4.41124	4.42200	
4d'	² P	1/2	4.40367	4.42950	
		3/2	4.41124	4.42200	
		5/2	4.41937		
		7/2	4.41512		
		3/2	4.43622		
4d	⁴ D	1/2	4.44430		
		9/2	4.44882		
		7/2	4.47484		
		5/2	4.47047		
		3/2	4.47607		
4d'	² D	5/2	4.45567	4.44700	
		3/2	4.46532	4.45300	
4d	² F	7/2	4.45014		
		5/2	4.49028		
4d	⁴ P	1/2	4.48405		
		3/2	4.49092		
		5/2	4.50316		
4d	² P	1/2	4.50531		
		3/2	4.50916		
4d'	² G	7/2	4.57535		
		9/2	4.57722		
4d'	² F	5/2	4.61416		
		7/2	4.61716		

Fine-structure energy levels – Cr VIII ion

Table 5. Comparison of oscillator strengths for the transitions listed in the table against the results of Fawcett [4] and others.

Upper level	Term	J	Lower level – $3s^23p^5$ ($^2P_{3/2}^o$)		Lower level – $3s^23p^5$ ($^2P_{1/2}^o$)	
			f_t		f_t	
			Present	Others	Present	Others
$3s3p^6$	2S	1/2	0.20352(–01)	0.17250(–01) 0.24975(–01) ^a 0.25575(–01) ^b	0.02045	0.01750 0.0254 ^a 0.02565 ^b
3d	4D	5/2	0.19998(–05)		0.12931(–04)	
		3/2	0.48481(–05)			
		1/2	0.85762(–05)		0.27118(–04)	
3d'	2P	3/2	0.15886(–03)	0.00275	0.76583(–03)	
		1/2	0.24851(–03)		0.19512(–02)	
3d	4F	5/2	0.18123(–03)			
		3/2	0.82292(–05)		0.11743(–04)	
3d'	2D	3/2	0.28197(–02)		0.10812(–01)	
		5/2	0.12197(–01)			
3d	4P	1/2	0.60869(–03)		0.23988(–03)	
		3/2	0.17192(–03)		0.25352(–03)	
		5/2	0.65821(–04)			
3d	2F	5/2	0.17866(–03)			
3d'	2F	5/2	0.71719(–03)			
3d''	2D	3/2	0.10525(–02)		0.64939(–02)	0.85000(–02)
		5/2	0.17047(–03)			
3d'	2S	1/2	0.37922	0.40600	0.28391	0.26300
3d	2P	3/2	0.83900	1.06150	0.76551(–01)	1.16000(–01)
		1/2	0.11876	0.1425	0.64473	0.83300
3d	2D	5/2	1.50740	1.73475		
		3/2	0.05569	0.06400	0.18817(+01)	0.21715(+01)
4s	4P	5/2	0.15762(–02)			
		3/2	0.01718	0.02800	0.16552(–02)	
		1/2	0.27984(–02)		0.88357(–03)	
4s	2P	3/2	0.11490	0.14200	0.23530(–01)	0.29500(–01)
		1/2	0.02725	0.03850	0.89035(–01)	1.12500(–01)
4s'	2D	5/2	0.07696	0.09725		
		3/2	0.35084(–03)		0.11473	0.14000
4s''	2S	1/2	0.01505	0.01750	0.29488(–01)	0.37500(–01)
3p ⁶ 3d	2D	3/2	0.10864(–06)		0.34022(–05)	
		5/2	0.13213(–04)			
4d	2D	5/2	0.14154			
		3/2	0.19894(–01)		0.10328	
4d'	2S	1/2	0.20113(–01)		0.17129(–01)	
4d'	2P	1/2	0.44255(–02)		0.64770(–02)	
		3/2	0.24145(–01)		0.10677(–02)	
4d	4D	5/2	0.14185(–01)			
		3/2	0.69790(–02)		0.43460(–01)	
		1/2	0.13294(–02)		0.37288(–02)	

Table 5. *Continued.*

Upper level	Term	J	Lower level – $3s^23p^5$ ($^2P_{3/2}^o$)		Lower level – $3s^23p^5$ ($^2P_{1/2}^o$)	
			f_l		f_l	
			Present	Others	Present	Others
4d	4F	5/2	0.37183(-02)			
		3/2	0.31859(-05)		0.61384(-03)	
4d'	2D	5/2	0.22146(-01)			
		3/2	0.37410(-02)		0.72678(-01)	
4d	2F	5/2	0.20321(-02)			
4d	4P	1/2	0.14103(-03)		0.59299(-02)	
		3/2	0.17349(-02)		0.20640(-02)	
		5/2	0.30103(-02)			
4d	2P	1/2	0.11482(-01)		0.61499(-01)	
		3/2	0.52758(-01)		0.13963(-01)	
4d'	2F	5/2	0.46356(-03)			

^aBPW [5]; ^bBT [6].

Table 6. Calculated transition probabilities and lifetimes for the transitions listed in the table.

Upper level	Term	J	Lower Level –	Lower level –	Lifetime (ns)
			$3s^23p^5$ ($^2P_{3/2}^o$)	$3s^23p^5$ ($^2P_{1/2}^o$)	
			A_l	A_l	τ
3s3p ⁶	2S	1/2	0.15334(10)	0.70573(9)	0.447
3d	4D	5/2	0.96268(5)		0.104(5)
		3/2	0.35144(6)	0.44011(6)	0.126(4)
		1/2	0.12498(7)	0.18557(7)	0.322(3)
3d'	2P	3/2	0.13552(8)	0.30828(8)	0.225(2)
		1/2	0.42405(8)	0.15711(9)	0.501(1)
3d	4F	5/2	0.10576(8)		0.946(2)
		3/2	0.72458(6)	0.48833(6)	0.824(3)
3d'	2D	3/2	0.25287(9)	0.45820(9)	0.141(1)
		5/2	0.75156(9)		0.133(1)
3d	4P	1/2	0.11168(9)	0.20810(8)	0.755(1)
		3/2	0.15984(8)	0.11150(8)	0.369(2)
		5/2	0.41456(7)		0.241(3)
3d	2F	5/2	0.11873(8)		0.842(2)
3d'	2F	5/2	0.54569(8)		0.183(2)
3d''	2D	3/2	0.13546(9)	0.39871(9)	0.187(1)
		5/2	0.14812(8)		0.675(2)
3d'	2S	1/2	0.10984(12)	0.39335(11)	0.670(-2)
3d	2P	3/2	0.13161(12)	0.57538(10)	0.728(-2)
		1/2	0.38852(11)	0.10116(12)	0.714(-2)

Table 6. Continued.

Upper level	Term	J	Lower Level –	Lower level –	Lifetime (ns)
			$3s^23p^5(^2P_{3/2}^o)$	$3s^23p^5(^2P_{1/2}^o)$	
			A_l	A_l	τ_l
3d	2D	5/2	0.16277(12)		0.614(–2)
		3/2	0.93367(10)	0.15137(12)	0.622(–2)
4s	4P	5/2	0.38001(9)		0.263(1)
		3/2	0.63011(10)	0.29523(9)	0.152
		1/2	0.21550(10)	0.33113(9)	0.402
4s	2P	3/2	0.43126(11)	0.42964(10)	0.211(–1)
		1/2	0.20779(11)	0.33033(11)	0.186(–1)
4s'	2D	5/2	0.20300(11)		0.493(–1)
		3/2	0.13892(9)	0.22116(11)	0.449(–1)
4s''	2S	1/2	0.13082(11)	0.12490(11)	0.391(–1)
3p ⁶ 3d	2D	3/2	0.61622(5)	0.94365(6)	0.995(3)
		5/2	0.50150(7)		0.199(3)
4d	2D	5/2	0.56728(11)		0.176(–1)
		3/2	0.11976(11)	0.30420(11)	0.236(–1)
4d'	2S	1/2	0.24934(11)	0.10394(11)	0.283(–1)
4d'	2P	1/2	0.55149(10)	0.39508(10)	0.106
		3/2	0.15096(11)	0.32678(9)	0.648(–1)
4d	4D	5/2	0.59230(10)		0.169
		3/2	0.44130(10)	0.13454(11)	0.560(–1)
		1/2	0.16874(10)	0.23171(10)	0.250
4d	4F	5/2	0.15917(10)		0.628
		3/2	0.20509(7)	0.19349(9)	0.511(1)
4d'	2D	5/2	0.94174(10)		0.106
		3/2	0.23966(10)	0.22798(11)	0.397(–1)
4d	2F	5/2	0.87765(9)		0.114(1)
4d	4P	1/2	0.18222(9)	0.37518(10)	0.254
		3/2	0.11242(10)	0.65497(9)	0.562
		5/2	0.13076(10)		0.765
4d	2P	1/2	0.14977(11)	0.39284(11)	0.184(–1)
		3/2	0.34466(11)	0.44672(10)	0.257(–1)
4d'	2F	5/2	0.21140(9)		0.473(1)

In table 4 we have also compared our results with the calculations of Fawcett [3]. In his calculations, Fawcett has used least-square fitting technique to adjust the energies to the experimental results so that the differences between his adjusted energies (shown in table 4) and experimental results are minimum while our results shown in table 4 involves a large number of configurations.

The oscillator strengths of E1 transitions are shown in table 5 in the length form. In table 6 we have presented our calculated transition probabilities and lifetimes of the even parity levels. Only the length form is used. For strong transitions, there is a good agreement between the length and the velocity forms. For transitions subject to cancellation due to CI effects, the length value is normally more stable with respect to the addition of further configurations. For transitions which are

forbidden in LS coupling, Drake [13] has shown that the length form is the correct one to use, whereas the velocity operator requires a relativistic correction.

Lastly we would like to add that we have predicted many new lines up to $3p^4(^1D)4d\ ^2F$ levels which have not been predicted so far either experimentally or theoretically. We expect our results to be accurate, as we have taken all the important correlations and relativistic effects in our calculations.

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