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Collisional excitation among the seven lowest states of TiXII

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Abstract. Collision strengths have been calculated for electron impact excitation of sodium-like TiXII for all 21 transitions amongst its lowest seven states. Configuration interaction wave functions have been used to represent the target states. The standard and no-exchange R-matrix codes have been used to calculate the contribution of partial waves with $L \leqslant 8$ and $L > 8$ respectively. Collision strengths are tabulated at selected energies in the range 26 to 50 Ryd. Effective collision strengths are tabulated for electron temperatures in the range $\log T_e = 4{\cdot}0$ to $\log T_e = 6{\cdot}0$, with T_e in K. This is the first detailed calculation on this ion in which the effects of exchange, channel couplings and short-range correlation are taken into account.

Keywords. Collision strength; R-matrix method.

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1. Introduction

The spectra and term systems of Na-like ions have been extensively studied over the years [1]. Recently there has been renewed interest in Na-like ions because they have proved to be a useful tool in diagnosing fusion plasmas, since their spectral lines are rather strong and easy to identify. TiXII is one of the most important constituents on the Tokamak plasma since Ti is present as a metallic impurity in the fusion reactor and is responsible for the radiative power loss from the plasma [2].

In the area of X-ray laser research, Na-like ions play an important role in understanding the lasing action in Na-like ions in an electron collision excitation scheme which has been utilized successfully in the recent work of many groups (Matthews *et al* [3], Fields *et al* [4]).

The spectrum of TiXII was first observed by Edlen [5]. Ekberg and Svensson [6] and Cohen and Behring [7] extended the analysis of the series of transitions $3s - np$, $3p - ns$, $3p - nd$ and $3d - nf$ up to $11p$, $7s$, $10d$ and $8f$. Recently, Westerlind [8] has recorded a new spectra of highly ionized Ti in the wavelength regions 335–1165Å and 1300 –1400 Å using the beam-foil technique. The term system has been extended to include all configurations up to $8f$, with the exception of $8s$. In addition, Zhang *et al* [9] have reported collision strengths for several Na-like ions using the distorted wave method.

In the present work, we have used the R-matrix method (Burke and Robb [10]) in a manner similar to that of Dufton and Kingston [11] and Mohan *et al* [12].

This method permits the explicit inclusion of the effects of resonances converging to all target states included in the calculation. We have performed a seven-state close-coupling LS calculation in which the target states are represented by configuration interaction wave functions determined using the CIV 3 code [13].

The collision strengths, Ω, have been computed at a large number of electron incident energies and tabulated at selected values in the range 26 to 50 Ryd. Further, the Ω's are integrated over a Maxwellian distribution of electron velocities to obtain the effective collision strengths γ which are tabulated in the electron temperature range of log $T_e = 4{\cdot}0$ to $6{\cdot}0$ K. These are the first detailed calculations of Ω and γ for this ion in which the important physical effects of exchange, channel coupling and short range correlation have properly been taken into account.

2. Calculations

Using the CIV3 code, Hibbert *et al* [14] have recently calculated configuration–interaction (CI) wave functions for Na-like ions, including TiXII. The CI wave function in LS coupling is represented by an expansion of the form

$$\psi(LS) = \sum_{i=1}^{k} a_i \Phi_i(\alpha_i LS), \tag{1}$$

where $\{\Phi_i\}$ are configuration state functions constructed from one-electron orbitals whose angular momenta are coupled as specified by $\{\alpha_i\}$ to form a total L and S common to all configurations. The radial part of each orbital is written as a linear combination of normalized Slater-type orbitals

$$P_{nl}(r) = \sum_{j=1}^{k} c_{jnl} \left[\frac{(2\zeta)^{2I_{jnl}+1}}{(2I_{jnl})!} \right]^{1/2} r^{I_{jnl}} \exp(-\zeta_{jnl} r) \tag{2}$$

with

$$\int_0^\infty P_{nl}(r) P_{n'l}(r)\, \mathrm{d}r = \delta_{nn'}.$$

The parameters $\{a_i\}$ in (1) and the parameters in (2) were determined variationally by Hibbert *et al* [14]. The 1*s*, 2*s*, 2*p* and 3*s* functions were chosen as the Hartree–Fock orbitals of the ^2S ground state of TiXII (Clementi and Roetti [15]). The remaining orbitals P_{nl} were optimized on the energies of the respective excited states $1s^2 2s^2 2p^6 nl^2 L$.

In table 1, we list the optimized radial function parameters used in (2) for the 4*s*, 3*p*, 4*p*, 3*d*, 4*f* orbitals. Table 2 lists the configurations used to generate the seven target states which are indexed in table 3 in order of increasing energy. The choice of configurations includes some allowance for core polarization, through using the valence orbitals rather than correlation orbitals optimized specifically for this purpose so as to retain a fairly simple target wave functions. Nevertheless, there is satisfactory agreement between our calculated energies and the experimental values given by Corliss and Sugar [16].

The total wave function for TiXII plus an electron is expressed as an R-matrix expansion, as discussed by Burke and Robb [10] and by Mohan [12]. The R-matrix

Table 1. Radial function parameters.

Orbital	I_{jnl}	C_{jnl}	ξ_{jnl}
4*s*	1	0·11185	17·22634
	2	−0·59853	6·61167
	3	2·04148	3·89881
	4	−2·17776	3·33069
3*p*	2	0·49399	8·85806
	3	−1·10311	4·23216
4*p*	2	0·33946	8·62129
	3	−2·69541	3·17489
	4	3·01155	3·20437
3*d*	3	1·00000	4·38539
4*d*	3	0·79541	4·41103
	4	−1·27383	2·84074
4*f*	4	1·00000	3·01680

Table 2. Target state configurations.

Target state	State number	Configurations
^2S	1·4	$[1s^22s^2]$ $2p^63s$, $2p^64s$, $2p^53p3s$, $2p^53p4s$ $2p^53d3p$, $2p^53d4p$
$^2P^0$	2·5	$[1s^22s^2]$ $2p^63p$, $2p^64p$, $2p^53p^2$, $2p^53p4p$, $2p^53s3d$
^2D	3·6	$[1s^22s^2]$ $2p^63d$, $2p^64d$, $2p^53p3d$, $2p^54p3d$, $2p^53p4d$
$^2F^0$	7	$[1s^22s^2]$ $2p^64f$, $2p^53p^2$, $2p^53p4p$, $2p^53d^2$

Table 3. Energy threshold relative to the ground state.

		Energies (Ryd)	
Key	State	Theoretical[a]	Experimental[b]
1	$1s^22s^22p^63s$ ^2S	0·00000	0·00000
2	$1s^22s^22p^63p$ $^2P^0$	1·90683	1·95153
3	$1s^22s^22p^63d$ ^2D	4·52602	4·57873
4	$1s^22s^22p^64s$ ^2S	10·24579	10·32988
5	$1s^22s^22p^64p$ $^2P^0$	10·98815	11·08645
6	$1s^22s^22p^64d$ ^2D	11·93488	12·04416
7	$1s^22s^22p^64f$ $^2F^0$	12·26882	12·39689

[a]This work, CI wave functions.
[b]Corliss and Sugar [16], averaged over fine structure levels.

packages of Berrington *et al* [17] were used in the present work. We have included 20 continuum orbitals for each angular momentum of the continuum electron having maximum energy up to 60 Ryd which ensure convergence in the energy range considered here. We imposed a zero logarithmic derivative at the R-matrix boundary radius of 6·0 a.u.

For the inner region ($r < 6{\cdot}0$ a.u.) we included all the short range $(N+1)$-electron correlation terms which could be constructed from the bound orbitals to take account of the channels which would otherwise be omitted.

In the outer region ($r > 6{\cdot}0$ a.u.), the coupled differential equations are solved using the asymptotic code based on the method of Seaton [17]. This treats multipole coupling by first-order perturbation theory. The LS coupled K-matrices, obtained by matching the inner and outer region solutions at the R-matrix boundary, were used to calculate the collision strengths. We have considered all partial waves up to the $(N+1)$-electron angular momentum $L = 8$ for both parities and spin multiplicities (singlet and triplet). This was sufficient to obtain converged results for forbidden transitions. However, for allowed transitions it was necessary to include the contribution of higher partial waves for convergence to be achieved. Since exchange effects were found to be negligible for $L \geq 10$, a non-exchange R-matrix approximation, which amounts to neglecting the antisymmetrization and the bound type part of R-matrix expansion [10], is sufficient for higher partial waves [18]. A fast no-exchange R-matrix code (NERM) recently developed by Burke *et al* [19], has therefore been used to calculate the contribution from $L = 10$ to 40 and, finally, a 'top up' procedure, based on the sum rule of Burgess *et al* [20], which accounts approximately for $L > 40$.

3. Collision strengths and rate coefficients

In order to determine the resonances in Ω, we have undertaken calculations at a large number of incident electron energies, particularly in the threshold energy region. An energy mesh of 0·001 Ryd has been used at energies close to threshold but has gradually been increased with increasing incident energy. To give an idea of the energy density of the calculations, we show in figure 1 the variation of Ω with incident electron energy. It is clear that the collision strengths are dominated by closed-channel (Feshbach) resonances throughout the threshold energy region. These resonances converge to higher thresholds and contribute significantly to our calculations of effective collision strengths.

In table 4 we list our collision strengths (Ω) for 21 transitions involving the seven lowest states, at selected energy points. These are the first close-coupling results for collision strengths among these excited states. Zhang *et al* [8] have performed distorted wave (DW) calculations, but for inner-shell transitions ($2s^2 2p^6 3l \rightarrow 2s^2 2p^5 3l3l'$, $2s^2 2p^6 3l \rightarrow 2s2p^6 3l3l'$), so comparison with our calculations is not possible.

Since the excitation collision strengths vary rapidly with energy in the threshold region, it is not practicable to tabulate them. However, for many plasma applications, excitation rate coefficients rather than the collision strengths are needed. They are obtained by integrating the collision strengths over a Maxwellian distribution of incident electron energies. This is the usual distribution of electron velocities for astrophysical applications but any other distribution can be examined using our

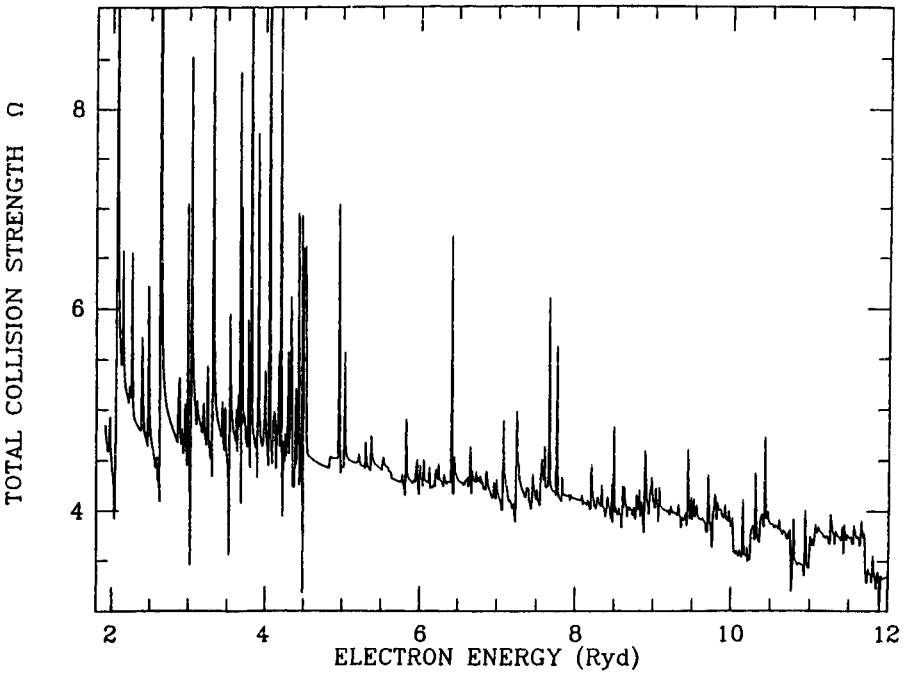

Figure 1. Energy variation of the total collision strengths for $1s^2 2s^2 2p^6 3s\ ^2S^e \rightarrow 1s^2 2s^2 2p^6\ ^2P^0$ allowed transition in TiXII.

Ω tabulated in table 4. The excitation rate coefficient (Eissner and Seaton [21]) for transition i to f at an electron temperature T_e is given by

$$C_{i,f} = \frac{8{\cdot}63 \times 10^{-6}}{g_i T^{1/2}} \gamma_{i,f} \exp\left[\frac{-\Delta E_{if}}{kT_e}\right] \mathrm{cm^3 s^{-1}}, \tag{3}$$

where $g_i = (2L_i + 1)(2S_i + 1)$ is the statistical weight of the lower state i, $\Delta E_{if} = E_f - E_i$ is the excitation energy and $\gamma_{i,f}$ defined as

$$\gamma_{i,f} = \int_0^{-\infty} \Omega(i \rightarrow f) \exp(-E_f/kT_e)\, \mathrm{d}(E_f/kT_e) \tag{4}$$

is the effective (dimensionless) collision strength for the transition i to f, E_f is the energy of the incident electron with reference to upper level f and k is the Boltzmann constant. In table 5, we have given $\gamma_{i,f}$ for all transitions over the electron temperature range from $\log(T_e) = 4{\cdot}0$ to $\log(T_e) = 6{\cdot}0$ where T_e is in K.

In general the collision strengths Ω or the effective collision strengths γ were found to be larger for the dipole allowed transitions than for the forbidden transitions. For the transitions from the ground state, the strongest corresponds to the resonance transition $3s \rightarrow 3p$ $(1-2)$. Among the transitions from the first excited state, the largest Ω or γ was found for the $3p \rightarrow 3d$ $(2-3)$ transition, which is again dipole-allowed. Among all the transitions, the $4p \rightarrow 4d$ $(5-6)$ and $4d \rightarrow 4f$ $(6-7)$ are the strongest as expected.

Table 4. Collision strengths for transitions in TiXII in the energy range 26–50 Ryd ($a \pm b \equiv a \times 10^{\pm b}$).

Transition		Energy (Ryd)									
I	*J*	26·00	28·00	30·00	32·00	34·00	36·00	38·00	40·00	45·00	50·00
1	2	7·738 – 00	7·870 – 00	7·995 – 00	8·112 – 00	8·258 – 00	8·364 – 00	8·463 – 00	8·559 – 00	8·778 – 00	8·971 – 00
1	3	5·852 – 01	5·889 – 01	5·923 – 01	5·953 – 01	5·979 – 01	5·999 – 01	6·017 – 01	6·035 – 01	6·083 – 01	6·119 – 01
1	4	1·652 – 01	1·663 – 01	1·673 – 01	1·685 – 01	1·695 – 01	1·703 – 01	1·708 – 01	1·713 – 01	1·727 – 01	1·741 – 01
1	5	5·235 – 02	5·582 – 02	5·938 – 02	6·298 – 02	6·653 – 02	7·001 – 02	7·342 – 02	7·679 – 02	8·513 – 02	9·291 – 02
1	6	6·442 – 02	6·662 – 02	6·873 – 02	7·072 – 02	7·262 – 02	7·440 – 02	7·608 – 02	7·763 – 02	8·104 – 02	8·399 – 02
1	7	1·334 – 01	1·343 – 01	1·351 – 01	1·360 – 01	1·367 – 01	1·373 – 01	1·379 – 01	1·384 – 01	1·395 – 01	1·404 – 01
2	3	1·178 + 01	1·201 + 01	1·223 + 01	1·244 + 01	1·264 + 01	1·282 + 01	1·300 + 01	1·317 + 01	1·361 + 01	1·400 + 01
2	4	1·273 – 01	1·344 – 01	1·417 – 01	1·491 – 01	1·565 – 01	1·637 – 01	1·709 – 01	1·781 – 01	1·963 – 01	2·134 – 01
2	5	6·664 – 01	6·713 – 01	6·760 – 01	6·811 – 01	6·862 – 01	6·908 – 01	6·948 – 01	6·982 – 01	7·063 – 01	7·141 – 01
2	6	3·438 – 01	3·635 – 01	3·832 – 01	4·029 – 01	4·224 – 01	4·415 – 01	4·599 – 01	4·779 – 01	5·216 – 01	5·629 – 01
2	7	7·923 – 01	8·126 – 01	8·321 – 01	8·503 – 01	8·671 – 01	8·825 – 01	8·969 – 01	9·107 – 01	9·426 – 01	9·678 – 01
3	4	7·425 – 02	7·621 – 02	7·826 – 02	8·034 – 02	8·243 – 02	8·446 – 02	8·642 – 02	8·827 – 02	9·244 – 02	9·583 – 02
3	5	2·919 – 01	3·017 – 01	3·120 – 01	3·230 – 01	3·344 – 01	3·456 – 01	3·569 – 01	3·681 – 01	3·969 – 01	4·249 – 01
3	6	1·326 – 00	1·324 – 00	1·322 – 00	1·322 – 00	1·324 – 00	1·325 – 00	1·326 – 00	1·327 – 00	1·331 – 00	1·335 – 00
3	7	6·107 – 00	6·348 – 00	6·578 – 00	6·798 – 00	7·008 – 00	7·211 – 00	7·407 – 00	7·596 – 00	8·037 – 00	8·439 – 00
4	5	3·005 + 01	3·084 + 01	3·156 + 01	3·222 + 01	3·282 + 01	3·338 + 01	3·390 + 01	3·438 + 01	3·550 + 01	3·648 + 01
4	6	2·720 – 00	2·725 – 00	2·726 – 00	2·723 – 00	2·717 – 00	2·710 – 00	2·701 – 00	2·691 – 00	2·664 – 00	2·635 – 00
4	7	4·363 – 01	4·354 – 01	4·349 – 01	4·345 – 01	4·345 – 01	4·345 – 01	4·344 – 01	4·345 – 01	4·350 – 01	4·354 – 01
5	6	5·377 + 01	5·540 + 01	5·685 + 01	5·819 + 01	5·940 + 01	6·052 + 01	6·155 + 01	6·253 + 01	6·473 + 01	6·671 + 01
5	7	3·619 – 00	3·613 – 00	3·607 – 00	3·599 – 00	3·591 – 00	3·582 – 00	3·573 – 00	3·563 – 00	3·539 – 00	3·515 – 00
6	7	7·728 + 01	7·922 + 01	8·100 + 01	8·267 + 01	8·422 + 01	8·569 + 01	8·707 + 01	8·838 + 01	9·138 + 01	9·408 + 01

Table 5. Effective collision strengths for transitions in TiXII ($a \pm b \equiv a \times 10^{\pm b}$).

Transition		Temperature (log K)										
I	J	4·0	4·20	4·40	4·60	4·80	5·00	5·20	5·40	5·60	5·80	6·00
1	2	4·850 – 00	4·968 – 00	5·079 – 00	5·144 – 00	5·166 – 00	5·158 – 00	5·110 – 00	5·011 – 00	4·890 – 00	4·863 – 00	5·060 – 00
1	3	7·134 – 01	6·789 – 01	6·535 – 01	6·374 – 01	6·268 – 01	6·224 – 01	6·258 – 01	6·320 – 01	6·325 – 01	6·246 – 01	6·130 – 01
1	4	2·346 – 01	2·365 – 01	2·335 – 01	2·259 – 01	2·155 – 01	2·031 – 01	1·898 – 01	1·781 – 01	1·698 – 01	1·650 – 01	1·630 – 01
1	5	1·395 – 01	1·333 – 01	1·249 – 01	1·165 – 01	1·069 – 01	9·451 – 02	8·077 – 02	6·835 – 02	5·886 – 02	5·288 – 02	5·066 – 02
1	6	4·420 – 01	2·789 – 01	1·762 – 01	1·134 – 01	7·856 – 02	6·215 – 02	5·573 – 02	5·374 – 02	5·364 – 02	5·464 – 02	5·670 – 02
1	7	7·416 – 01	4·683 – 01	2·995 – 01	2·036 – 01	1·571 – 01	1·382 – 01	1·317 – 01	1·298 – 01	1·295 – 01	1·298 – 01	1·305 – 01
2	3	9·452 – 00	9·195 – 00	8·927 – 00	8·670 – 00	8·453 – 00	8·300 – 00	8·208 – 00	8·153 – 00	8·155 – 00	8·316 – 00	8·718 – 00
2	4	4·593 – 01	5·456 – 01	5·869 – 01	5·798 – 01	5·306 – 01	4·526 – 01	3·653 – 01	2·863 – 01	2·248 – 01	1·825 – 01	1·577 – 01
2	5	9·527 – 01	9·593 – 01	9·510 – 01	9·402 – 01	9·146 – 01	8·622 – 01	7·995 – 01	7·459 – 01	7·079 – 01	6·843 – 01	6·725 – 01
2	6	2·087 – 00	1·317 – 00	8·322 – 01	5·355 – 01	3·711 – 01	2·939 – 01	2·640 – 01	2·556 – 01	2·570 – 01	2·656 – 01	2·836 – 01
2	7	3·652 – 00	2·306 – 00	1·475 – 00	1·003 – 00	7·746 – 01	6·834 – 01	6·546 – 01	6·512 – 01	6·594 – 01	6·762 – 01	7·021 – 01
3	4	1·120 – 00	1·376 – 00	1·432 – 00	1·335 – 00	1·163 – 00	9·702 – 01	7·793 – 01	6·029 – 01	4·525 – 01	3·343 – 01	2·481 – 01
3	5	2·134 – 00	2·160 – 00	2·069 – 00	2·034 – 00	2·052 – 00	1·976 – 00	1·746 – 00	1·430 – 00	1·116 – 00	8·571 – 01	6·680 – 01
3	6	1·205 + 01	7·606 – 00	4·806 – 00	3·093 – 00	2·142 – 00	1·693 – 00	1·512 – 00	1·444 – 00	1·413 – 00	1·394 – 00	1·377 – 00
3	7	2·516 + 01	1·589 + 01	1·016 + 01	6·908 – 00	5·331 – 00	4·703 – 00	4·517 – 00	4·521 – 00	4·626 – 00	4·817 – 00	5·113 – 00
4	5	1·478 + 01	1·483 + 01	1·476 + 01	1·463 + 01	1·433 + 01	1·416 + 01	1·473 + 01	1·616 + 01	1·812 + 01	2·033 + 01	2·266 + 01
4	6	2·072 + 01	1·307 + 01	8·260 – 00	5·316 – 00	3·683 – 00	2·918 – 00	2·624 – 00	2·538 – 00	2·534 – 00	2·559 – 00	2·592 – 00
4	7	2·895 – 00	1·828 – 00	1·169 – 00	7·940 – 01	6·108 – 01	5·341 – 01	5·041 – 01	4·902 – 01	4·806 – 01	4·717 – 01	4·633 – 01
5	6	3·056 + 02	1·928 + 02	1·219 + 02	7·841 + 01	5·432 + 01	4·311 + 01	3·906 + 01	3·845 + 01	3·948 + 01	4·146 + 01	4·425 + 01
5	7	2·036 + 01	1·285 + 01	8·221 – 00	5·588 – 00	4·309 – 00	3·789 – 00	3·610 – 00	3·560 – 00	3·554 – 00	3·562 – 00	3·575 – 00
6	7	3·096 + 02	1·955 + 02	1·250 + 02	8·502 + 01	6·569 + 01	5·817 + 01	5·626 + 01	5·688 + 01	5·881 + 01	6·165 + 01	6·531 + 01

For the forbidden transitions, those involving promotion of orbitals within $\Delta n = 0$ have the largest Ω or γ: $4s\ ^2S - 4d\ ^2D$ and $4p\ ^2P^0 - 4f\ ^2F^0$. These strongest transitions will be very useful for intensity diagnostic purposes in Tokamak plasmas.

To conclude, we except our results to be quite reliable, as we have included all the important physical effects like exchange, channel coupling and short range correlations into our calculations. We have, however, not taken relativistic effects in our calculations which become important for members of higher Z.

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