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Dielectronic satellite spectra of hydrogenlike titanium

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Theoretical atomic parameters calculated with the Z-expansion method and with the multiconfiguration Thomas-Fermi model set were recently reported and used in the analyses of dielectronic satellite spectra of hydrogenlike titanium observed from the Princeton Large Torus tokamak discharges. A comparison of our calculations, based on the Hartree-Fock-Slater atomic model, with the other two theoretical results show reasonable agreement with $n=2$ satellites but systematic and sometimes significant differences are found for $n=3$ and 4 satellites.

Recently Bitter *et al.*[1] reported on high-resolution x-ray spectra obtained from tokamak discharges with central electron temperatures in excess of 2 keV on the Princeton Large Torus. In addition to the Lyman-α lines of Ti^{21+}, which are clearly resolved, many other lines corresponding to doubly excited heliumlike Ti^{20+} are also observed as satellite lines. These satellite lines arise from the radiative decay of states produced by dielectronic capture processes. Similar observations have been reported from other tokamak discharges,[2-5] laser-induced fusion devices,[6-9] and solar active regions and flares[10-15] for $10 \leq Z \leq 26$.

The relative intensities of these dielectronic satellite spectra compared to the Lyman-α lines have been recognized as a potential diagnostic tool for electron temperature and electron density in a plasma. For low-density plasmas the intensities of dielectronic satellite lines, i_d, relative to the intensity of the resonance lines (with the assumption of a Maxwellian energy distribution for the electrons) can be expressed [see Eq. (2) of Ref. 1] as

$$i_d = \frac{2.619\times10^{-27}}{T_e^{3/2} C_R(T_e)} \exp\left(\frac{-E_s^n}{T_e}\right) F_2(s) ,$$

where T_e is the electron temperature in keV, $C_R(T_e)$ is the total collisional excitation rate for $1s$-$2p$ excitations (in $cm^3 sec^{-1}$), and

$$F_2(s) = g_s \frac{A_a(s) A_r(s)}{A_a(s) + \sum_{s'} A_r(s')} . \quad (1)$$

We use the same notation as in Ref. 1.

Clearly one of the important atomic parameters is F_2 for various transition arrays. Bitter *et al.*[1] presented theoretical values of F_2 with two different models: the Z-expansion method which is described in detail elsewhere[16] and the multiconfiguration Thomas-Fermi model.[15,17] The appropriate autoionization and radiative transition probabilities are calculated using these procedures, and F_2 values are obtained from Eq. (1). There are differences in the values of F_2 in many cases in these two theoretical calculations, in particular for $n > 2$ satellites.

We have performed similar calculations in which the Hartree-Fock-Slater atomic model[18,19] (HFS) is used. Each level, with quantum numbers, total energy, total angular momentum J, and parity, is expressed as a linear combination of basis functions with the same J and parity. The mixing of other configurations is restricted to the same complex. The total energies include relativistic corrections. The mixing coefficients are obtained by diagonalizing the Hamiltonian. Radiative and autoionization transition probabilities are then calculated numerically. The transition energies are obtained by taking the difference between the total energy of the initial level and the total energy of the final level. All levels of the doubly excited heliumlike titanium were considered for $n=2$ to $n=4$ satellites.

The purpose of this Rapid Communication is to present our F_2 values for strong dielectronic satellite lines and a comparison of these values with results obtained by the Z-expansion method and the scaled Thomas-Fermi model (TF) for titanium.[1]

Table I contains such a comparison for $n=2$ satellite lines, which are listed in the order of decreasing values of F_2. It is to be noted that the Z-expansion method gives higher F_2 values than the HFS values in contrast to consistently lower F_2 values of TF compared to the HFS results. The HFS values of F_2 are in reasonable agreement (within 7%) with the TF values, and with the Z-expansion F_2 values except in those cases when autoionization transition rates are nonzero only when the effects of the spin-orbit coupling and the electron configuration mixing are included, for example, $2p^2\,{}^3P_J$ levels.

The values of autoionization rates for $n=2$ states calculated with the HFS model lie between the corresponding values obtained with the Z-expansion method and with TF. The HFS wavelengths exhibit the same behavior indicating that the Z-expansion method incorporates "too little" atomic screening compared to HFS and the Thomas-Fermi scaled procedure slightly overestimates screening for $n=2$ satellites.

A comparison of theoretical F_2 values is presented in Table II for some transition arrays for initial configurations $2p\,np$, $2p\,ns$, and $2p\,nd$ with $n=3$ and 4. The listed electron configurations, and the L and S values designated by the spectroscopic notation, should be used only as a *guide* since the effects of electron configuration and spin-orbit mixing are significant in many cases. This is true in general in all three theoretical calculations. These cases were chosen since in each case one would have a spectator electron (np, or ns or nd) with the $2p$ to $1s$ x-ray transition

TABLE I. Theoretical values of F_2 (in units of 10^{13} s^{-1}) with the Hartree-Fock-Slater model (HFS), and percentage differences from values obtained with the Z-expansion method and with using the multiconfiguration Thomas-Fermi model (TF) for the $n=2$ satellite lines of the Ly-α lines of Ti XXII.

Array	F_2 (HFS)	% Difference[a]	% Difference[b]
$1s2p(^1P_1)$-$2p^2(^1D_2)$	64.77	0.6	−6.8
$1s2s(^1S_0)$-$2s2p(^1P_1)$	23.51	6.3	−5.2
$1s2p(^3P_2)$-$2p^2(^3P_2)$	14.4	17	−6.4
$1s2p(^3P_2)$-$2p^2(^1D_2)$	8.46	19	−6.9
$1s2p(^3P_1)$-$2p^2(^3P_2)$	6.3	22	−6.5
$1s2s(^3S_1)$-$2s2p(^3P_2)$	6.11	1.6	−3.8
$1s2s(^3S_1)$-$2s2p(^3P_1)$	4.21	5.2	−3.8
$1s2p(^1P_1)$-$2s^2(^1S_0)$	3.56	0.6	−2.0
$1s2p(^1P_1)$-$2p^2(^1S_0)$	2.52	5.9	−4.0
$1s2p(^1P_1)$-$2p^2(^3P_2)$	1.97	42	−9.6
$1s2s(^3S_1)$-$2s2p(^3P_0)$	1.22	1.6	−2.5
$1s2p(^3P_1)$-$2s^2(^1S_0)$	1.02	16	−6.9

[a] $100[F_2(Z\text{-expansion})-F_2(\text{HFS})]/F_2(\text{HFS})$. [b] $100[F_2(\text{TF})-F_2(\text{HFS})]/F_2(\text{HFS})$.

if the description of each state could be described accurately by a *single* electron configuration.

Table III contains the autoionization rates for the levels listed in Table II. It is clear that there is no simple procedure for extrapolation of autoionization rates (and F_2) from the values of $n=2$, 3, 4, and 5 for higher n values for all these satellites. Consequently, caution should be exercised in arriving at the possible corrections to the intensity of the resonance line resulting from the unresolved satellites for large n.

The Thomas-Fermi model gives consistently smaller values of F_2 for all $n=3$ and $n=4$ transition arrays in Table II. Unlike the differences in Table I, these discrepancies of TF from the HFS results are much greater and, therefore, significant. One reason for these deviations may be that the scaled Thomas-Fermi parameters are adjusted for each l value after minimization of energies of preselected states. The parameter obtained for each l value is then used for all n values. It is likely that the optimization of the parameters was performed for some states listed in Table I (and as a result the differences of TF and HFS are ≈ 2–7%); but as a consequence leading to possibly inaccurate descriptions of many states with an electron in $n \geq 3$.

The Z-expansion method involves a description of states that is accurate in the limit of large-Z value. However, where effects due to atomic screening and configuration mixing are not negligible (as is the case for states in Table

TABLE II. Theoretical values of F_2 (in units of 10^{13} s^{-1}) with the Hartree-Fock-Slater model (HFS) and percentage differences from values obtained with the Z-expansion method and with using the multiconfiguration Thomas-Fermi model (TF) for $n=3$ and $n=4$ strong satellite lines of Ly-α lines of Ti XXII. Transitions with F_2 values less than 10^{12} s^{-1} are not listed.

		$n=3$			$n=4$	
Array	F_2(HFS)	% Diff.[a]	% Diff.[b]	F_2(HFS)	% Diff.[a]	% Diff.[b]
$1snp(^1P_1)$-$2pnp(^1D_2)$	22.7	−9	−22	15.8	−29	−47
$(^3P_1)$- $(^3D_2)$	1.01	3	−53	1.40	−46	−84
$(^3P_2)$- $(^3D_3)$	0.96	1	−16	1.08	[c]	[c]
$1sns(^1S_0)$-$2pns(^1P_1)$	9.45	12	−19	4.6	18	−17
$(^3S_1)$- $(^3P_1)$	1.01	11	−2			
$(^3S_1)$- $(^1P_1)$	0.93	−1	−42	1.33	5	−22
$1snd(^1D_2)$-$2pnd(^1F_3)$	6.97	23	−16	5.94	−51	−55
$(^3D_2)$- $(^1F_3)$	3.48	36	−14	0.35		
$(^3D_3)$- $(^3F_4)$	4.05	15	−11	2.22	−10	−22
$(^3D_1)$- $(^3D_1)$	1.67	−67	−61			
$(^3D_3)$- $(^3F_3)$	1.22	20	−20			
$(^1D_2)$- $(^3F_3)$	1.12	26	−13			
$(^3D_2)$- $(^3F_3)$	0.95	6	−3	1.27	[c]	[c]

[a] $100[F_2(Z\text{-expansion})-F_2(\text{HFS})]/F_2(\text{HFS})$.
[b] $100[F_2(\text{TF})-F_2(\text{HFS})]/F_2(\text{HFS})$.
[c] No entry listed.

TABLE III. Comparison of autoionization rates in units of 10^{13} s^{-1} calculated with the Hartree-Fock-Slater model (HFS), the Z-expansion method, and using the multiconfiguration Thomas-Fermi model (TF) for doubly excited heliumlike titanium.

Autoionizing state	$n=3$ HFS	$n=3$ Z-expansion	$n=3$ TF	$n=4$ HFS	$n=4$ Z-expansion	$n=4$ TF
$2pnp(^1D_2)$	11.6	11.1	8.97	5.15	4.72	3.37
$(^3D_2)$	0.31	0.62	0.27	0.47	0.80	0.22
$(^3D_3)$	0.175	0.18	0.15	0.057	[a]	[a]
$2pns(^1P_1)$	7.79	8.58	6.17	2.44	2.90	1.97
$(^3P_1)$	0.58	0.50	0.39	0.23	1.14	0.81
$2pnd(^1F_3)$	2.1	2.4	1.8	1.07	0.90	0.84
$(^3F_4)$	0.46	0.53	0.41	0.25	0.23	0.20
$(^3F_3)$	0.50	0.58	0.43	0.21	0.31	0.23
$(^3D_1)$	0.80	0.54	0.76	0.01	[a]	[a]

[a]No entry listed.

II), this method may not always lead to accurate values of autoionization and radiative transition probabilities and, therefore, of F_2.

It may be noted that the effects of configuration mixing for $n \geq 3$ states are quite involved and influence transition rates, and significant differences in many cases exist between the three calculations; but these differences may not be of serious consequence in the analysis of the recent experiment with the reported resolution for either plasma diagnostic or total-recombination-rate purposes.

Comprehensive and systematic calculations with the HFS atomic model have been completed for a large range of atomic numbers, and the results will be submitted for publication in the immediate future.

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