Heavy-particle excitation of fluorinelike Fe XVIII

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(Received 21 June 1993)

Cross sections and rate coefficients for excitation of the $2s^22p^5\,^2P_{3/2}-2s^22p^5\,^2P_{1/2}$ transition in fluorinelike Fe XVIII by proton (p), deuteron (d), triton (t), and α-particle (α) impact have been calculated using the close-coupled impact-parameter method. These data, in conjunction with R-matrix calculations of electron-impact excitation rates, are used to derive the theoretical emission line ratio $R=I(2s^22p^5\,^2P_{3/2}-2s^22p^5\,^2P_{1/2})/I(2s^22p^5\,^2P_{3/2}-2s2p^6\,^2S_{1/2})=I(974.8\ \text{Å})/I(93.4\ \text{Å})$ as a function of electron and heavy-particle number density, and electron and ion temperature, for values applicable to tokamak plasmas. A comparison of our results with observations of R from the JIPP T-II-U tokamak at the Institute of Plasma Physics, Nagoya, Japan, for which the plasma parameters have been independently determined, reveals excellent agreement between theory and experiment, with discrepancies of typically $\leq 10\%$. This provides observational support for the accuracy of the atomic data adopted in the line ratio calculations.

PACS number(s): 34.10.+x

I. INTRODUCTION

Emission lines arising from transitions in the fluorinelike ion Fe XVIII have been widely detected in the spectra of high-temperature laboratory and astrophysical plasmas [1–4]. Among the most frequently observed are the $^2P_{3/2}$-$^2P_{1/2}$ forbidden line within the $2s^22p^5$ ground state at 974.8 Å and the $2s^22p^5\,^2P_{3/2,1/2}-2s2p^6\,^2S_{1/2}$ allowed transitions at 93.9 and 103.9 Å, respectively. These lines may be used to infer the electron density of a plasma with $N_e\simeq10^{13}-10^{15}$ cm^{-3}, typical in tokamak plasmas, through the diagnostic ratio $R=I(2s^22p^5\,^2P_{3/2}-2s^22p^5\,^2P_{1/2})/I(2s^22p^5\,^2P_{3/2}-2s2p^6\,^2S_{1/2})$, due to the movement of the metastable $2s^22p^5\,^2P_{1/2}$ level towards Boltzmann equilibrium [5]. The theoretical determination of this ratio depends on the atomic data used, especially for the excitation rates among the relevant levels [6].

As noted by Bely and Faucher [7] and Keenan and Reid [8,9], excitation of $2s^22p^5\,^2P_{1/2}$ from $^2P_{3/2}$ by proton collisions is important for F-like ions such as Fe XVIII, and in fact dominates the total collision rate at high temperatures. In this paper we present reliable atomic data for heavy-particle excitation of $^2P_{3/2}$-$^2P_{1/2}$ in Fe XVIII, and use these results to derive R ratios applicable to the analysis of tokamak plasmas.

II. HEAVY-PARTICLE EXCITATION CROSS SECTIONS AND RATES

Cross sections and rate coefficients for excitation of the $2s^22p^5\,^2P_{3/2}-2s^22p^5\,^2P_{1/2}$ transition in fluorinelike Fe XVIII by proton (p), deuteron (d), triton (t) and α-particle (α) impact have been calculated using the close-coupled impact-parameter method [10]. As in the previous calculation of Keenan and Reid [11], we have used a formulation which is symmetrical with respect to channel velocities, and we have modified the interactions at short range to take account of penetration of the electron cloud of the ion [12]. However, whereas the previous work [11] only considered the states of the $2s^22p^5\,^2P$ term, in the present analysis we have also included the $2s2p^6\,^2S$ state, achieving this by means of a polarization potential [13]. The effect of the inclusion of the ^2S state is to reduce sub-

TABLE I. Cross sections (in atomic units) for excitation of the $2s^22p^5\,^2P_{3/2}-2s^22p^5\,^2P_{1/2}$ transition in Fe XVIII induced by collisions with protons (p), deuterons (d), tritons (t), or α-particles (α).

Barycentric impact energy (keV)	Cross sections p	d	t	α
0.7	3.62[−3][a]	1.20[−3]	5.25[−4]	
0.8	8.74[−3]	4.17[−3]	2.02[−3]	
0.9	1.64[−2]	1.04[−2]	6.19[−3]	
1.0	2.55[−2]	1.98[−2]	1.37[−2]	4.24[−4]
1.1	3.51[−2]	3.16[−2]	2.45[−2]	5.03[−4]
1.2	4.42[−2]	4.44[−2]	3.74[−2]	8.98[−4]
1.4	5.88[−2]	6.85[−2]	6.44[−2]	3.89[−3]
1.6	6.76[−2]	8.66[−2]	8.75[−2]	1.25[−2]
1.8	7.18[−2]	9.80[−2]	1.04[−1]	2.81[−2]
2.0	7.27[−2]	1.04[−1]	1.15[−1]	4.89[−2]
2.5	6.79[−2]	1.05[−1]	1.24[−1]	1.06[−1]
3.0	6.02[−2]	9.82[−2]	1.21[−1]	1.49[−1]
4.0	4.66[−2]	8.09[−2]	1.06[−1]	1.83[−1]
6.0	3.06[−2]	5.63[−2]	7.76[−2]	1.68[−1]
10.0	1.82[−2]	3.45[−2]	4.91[−2]	1.16[−1]
20.0	9.37[−3]	1.81[−2]	2.61[−2]	6.25[−2]
40.0	4.87[−3]	9.46[−3]	1.38[−2]	3.31[−2]

[a] $A[-B]$ implies $A\times10^{-B}$.

TABLE II. Rate coefficients (in $cm^3 s^{-1}$) for excitation of the $2s^22p^5\,{}^2P_{3/2}$–$2s^22p^5\,{}^2P_{1/2}$ transition in Fe XVIII by protons (p), deuterons (d), tritons (t), and α-particles (α).

	Rates			
Temperature (10^6 K)	p	d	t	α
1.5	2.29[−13][a]	1.03[−14]	5.68[−14]	1.50[−15]
2.0	9.85[−13]	5.41[−13]	3.39[−13]	1.70[−14]
2.5	2.50[−12]	1.56[−12]	1.06[−12]	8.66[−14]
3.0	4.78[−12]	3.25[−12]	2.33[−12]	2.78[−13]
3.5	7.70[−12]	5.59[−12]	4.17[−12]	6.66[−13]
4.0	1.11[−11]	8.48[−12]	6.52[−12]	1.32[−12]
5.0	1.87[−11]	1.54[−11]	1.24[−11]	3.56[−12]
6.0	2.66[−11]	2.30[−11]	1.92[−11]	7.12[−12]
7.0	3.42[−11]	3.08[−11]	2.64[−11]	1.19[−11]
8.0	4.13[−11]	3.83[−11]	1.16[−11]	1.76[−11]
10.0	5.33[−11]	5.19[−11]	4.71[−11]	3.07[−11]
12.0	6.27[−11]	6.32[−11]	5.88[−11]	4.50[−11]
16.0	7.54[−11]	7.97[−11]	7.69[−11]	7.27[−11]
20.0	8.25[−11]	9.02[−11]	8.93[−11]	9.68[−11]
25.0	8.71[−11]	9.81[−11]	9.94[−11]	1.21[−10]
30.0	8.89[−11]	1.02[−10]	1.06[−10]	1.39[−10]
40.0	8.88[−11]	1.05[−10]	1.12[−10]	1.63[−10]

[a] $A[-B]$ means $A\times10^{-B}$.

stantially the ${}^2P_{3/2}$-${}^2P_{1/2}$ cross section [12] with, for example, in the region of maximum cross section, our result differing from the data of Keenan and Reid [11] by more than 60%. Finally, the quantities that we required for the determination of the interaction matrix elements were deduced from Cheng, Kim, and Desclaux [14], and the excitation energies were from Reader and Sugar [15]. Table I shows the cross sections Q (in atomic units) for excitation of the Fe XVIII forbidden line transition.

The significance of including polarization effects in intramultiplet excitation collisions was noted by Heil and co-workers [16] in their work on proton excitation of O IV ($2p\,{}^2P$) and Fe XIV ($3p\,{}^2P$). These authors took a molecular approach to the proton-ion interaction and included a significant number of excited configurations of the ion as well as charge-transferred configurations to give accurate ${}^2\Pi$ and ${}^2\Sigma^+$ potential curves. In our calculation, the polarization is taken into account by the inclusion of the $2s2p^6\,{}^2S$ state alone. We believe that in the case of highly charged F-like ions, the major component of the polarization can be incorporated by a single state, because the next states that contribute to the polarization (i.e., states with configuration $2s^22p^43s$) have much larger excitation energies than $2s2p^6\,{}^2S$. In the present instance of Fe XVIII, the ratio of the excitation energies of the $2s^22p^43s\,{}^2P$ and $2s^22p^5\,{}^2P$ states is about 6. This is a rather singular feature of F-like systems (with atomic numbers $Z\geq20$), and one would not expect that a single state could, in general, give a good representation of the polarization.

Excitation rate coefficients were obtained by averaging the cross sections over a Maxwellian energy distribution at several temperatures. These are listed in Table II for the four perturbers. The calculated cross sections were supplemented at lower energies with cross sections calculated by a first-order theory [17], modified to take account of the polarization potential [18].

The proton excitation rates presented in Table II are more than a factor of 2.2 smaller than the results of Kastner and Bhatia [19], over the small temperature range for which they present results. These authors used an approximate semiempirical formula for the cross section as a function of energy. Keenan and Reid [11] did not include the effects of the ${}^2S$ state, and our proton excitation rates are 30% lower than their results at low temperatures and up to 36% lower at high temperatures. Similar discrepancies are found for the deuteron and triton excitation rates, but for the α-particle rates our results are up to 40% lower than those of Keenan and Reid [11].

III. DIAGNOSTIC APPLICATIONS

To illustrate the effects of the new heavy-particle excitation rates on diagnostic emission line ratios, we have calculated the ratio

$$R=I(2s^22p^5\,{}^2P_{3/2}-2s^22p^5\,{}^2P_{1/2})/I(2s^22p^5\,{}^2P_{3/2}-2s2p^6\,{}^2S_{1/2})=I(974.8\ \text{Å})/I(93.9\ \text{Å})\ .$$

Our model ion consisted of the $2s^22p^5\,{}^2P_{3/2}$, ${}^2P_{1/2}$, and $2s2p^6\,{}^2S_{1/2}$ levels, the energies of which were taken from Reader and Sugar [15]. Electron-impact excitation rates, calculated using the R-matrix code [20], were obtained from Mohan *et al.* [21,22], while for Einstein A coefficients the results of Mohan and Hibbert [23] and Mohan *et al.* [21] for the ${}^2S$-${}^2P$ and ${}^2P_{1/2}$-${}^2P_{3/2}$ transitions, respectively, were adopted. The ratio was calculat-

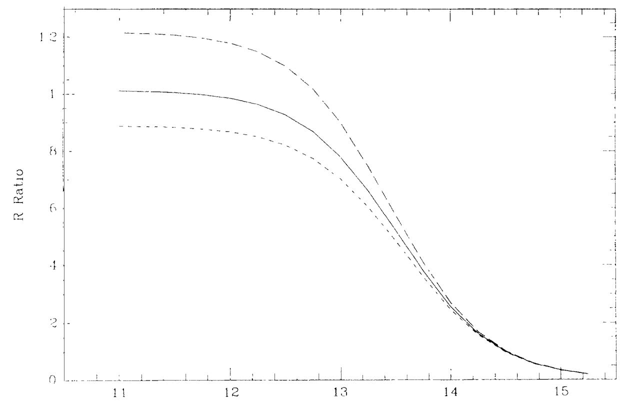

FIG. 1. The theoretical Fe XVIII emission line ratio (in photons) $R = I(2s^2 2p^5\,^2P_{3/2p} - 2s^2 2p^5\,^2P_{1/2})/I(2s^2 2p^5\,^2P_{3/2} - 2s 2p^6\,^2S_{1/2}) = I(974.8\ \text{Å})/I(93.9\text{Å})$ plotted as a function of electron density (N_e), with both proton- and electron-impact excitation rates included in the calculations. Results are given for three ion temperatures: T_{ion}, where $T_{\text{ion}} = 0.5T_e$ (short-dashed line), $T_{\text{ion}} = T_e$ (solid line), and $T_{\text{ion}} = 2T_e$ (long-dashed line), where T_e is the temperature of maximum Fe XVIII fractional abundance in ionization equilibrium, $T_{\max} = 5 \times 10^6$ K [24]. Note that the proton number density $N_p = N_e$.

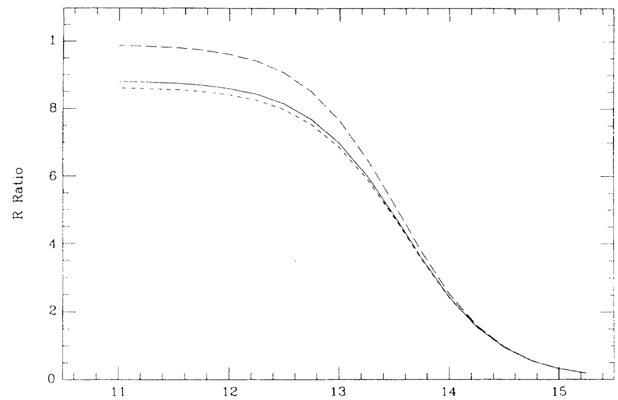

FIG. 2. The theoretical Fe XVIII emission line ratio (in photons) $R = I(2s^2 2p^5\,^2P_{3/2} - 2s^2 2p^5\,^2P_{1/2})/I(2s^2 2p^5\,^2P_{3/2} - 2s 2p^6\,^2S_{1/2}) = I(974.8\ \text{Å})/I(93.9\ \text{Å})$ plotted as a function of electron density (N_e), with both α-particle and electron-impact excitation rates included in the calculations. Results are given for three ion temperatures: T_{ion}, where $T_{\text{ion}} = 0.5T_e$ (short-dashed line), $T_{\text{ion}} = T_e$ (solid line), and $T_{\text{ion}} = 2T_e$ (long-dashed line), where T_e is the temeprature of maximum Fe XVIII fractional abundance in ionization equilibrium, $T_{\max} = 5 \times 10^6$ K [24]. Note that the α-particle number density $N_\alpha = 0.5N_e$.

ed for each of the heavy particles separately, and plotted as a function of electron density at $T_{\text{ion}} = T_{\max}$, $T_{\text{ion}} = 0.5T_{\max}$, and $T_{\text{ion}} = 2T_{\max}$, where $T_{\max} = 5 \times 10^6$ K is the temperature of maximum fractional abundance of Fe XVIII in ionization equilibrium [24].

Figures 1 and 2 show the R ratio as a function of electron density at ion temperatures of $T_{\text{ion}} = T_e = T_{\max}$, $T_{\text{ion}} = 0.5T_{\max}$, and $T_{\text{ion}} = 2T_{\max}$. In Fig. 1, the electron excitation rates are considered along with the proton excitation rates, while in Fig. 2 electron excitation rates and α-particle excitation rates are included. When deuteron and triton excitation rates were considered separately with electron excitation rates, they were found to lead to similar R ratios to the proton case. For the proton, deuteron, and triton particle cases we have assumed the heavy-particle number density to be equal to the electron density N_e, but for the α-particle case we took the number density to be $0.5N_e$, as would be expected for a pure α-particle plasma. It may be seen from Fig. 1 and 2 that the R ratio is strongly dependent on the magnitude of the heavy-particle excitation rates for the forbidden transition, and hence the ion temperature, especially when $T_{\text{ion}} > T_{\max}$, such as occurs during the rf heating of a tokamak discharge, as noted by Sato *et al.* [25]. Therefore our theoretically calculated line ratio may be used to determine the ion temperature of a plasma if the electron density and temperature have been independently determined, or alternatively one may obtain the electron density if the electron temperature and ion temperature are known. We note that the ratio

$$R' = I(2s^2 2p^5\,^2P_{3/2} - 2s^2 2p^5\,^2P_{1/2})/I(2s^2 2p^5\,^2P_{1/2} - 2s 2p^6\,^2S_{1/2}) = I(974.8\ \text{Å})/I(103.9\ \text{Å})$$

has the same density dependence as R but with $R' = 2.7R$, due to the common upper levels of the relevant transitions.

To examine the validity of our diagnostics, we have compared our theoretical line ratios with those measured by Sato *et al.* [25] during an ion-Bernstein-wave-heating (IBWH) experiment on the JIPP T-II-U tokamak at the Institute of Plasma Physics, Nagoya, Japan [26]. We considered only the theoretical ratio with proton collisions for this particular plasma. The plasma parameters before heating were the Ohmic current $I_p = 110$ kA, toroidal field $B_t = 18$ kG, electron density $N_e = 1.5 \times 10^{13}$ cm^{-3}, and electron temperature $T_e = 700$ eV. About 95 ms after the start of discharge, a 40-MHz rf pulse was applied of 80 kW for 30 ms. The time evolution of the line-averaged electron density was obtained using 2-mm mi-

TABLE III. Comparison of theoretical R ratios (R_{theory}) with those measured by Sato *et al.* [25] (R_{observed}) from the JIPP T-II-U tokamak. We note that for these observations the proton number density $N_p = N_e$.

Time/ms	T_i/keV	T_e/keV	N_e/cm^{-3}	R_{observed}	R_{theory}
75	0.33	0.45	1.50[+13][a]	0.36	0.58
85	0.30	0.50	2.25[+13]	0.40	0.57
95	0.35	0.65	2.25[+13]	0.45	0.54
100	0.50	0.70	2.25[+13]	0.58	0.57
105	0.60	0.75	2.25[+13]	0.69	0.58
110	0.90	0.80	2.25[+13]	0.68	0.63
115	0.87	0.65	2.25[+13]	0.65	0.64
120	0.85	0.62	2.25[+13]	0.59	0.64
125	0.84	0.60	2.25[+13]	0.53	0.64
135	0.45	0.58	1.57[+13]	0.46	0.57

[a] $A[+B]$ implies $A \times 10^B$.

crowave interferometry, the central electron temperature being measured by Thompson scattering, while the ion temperature was determined with a fast neutral energy analyzer. Sato *et al.* [25] derived their observed intensity ratios from the recorded time behavior of the Fe XVIII lines during the IBWH, and they claim that the uncertainty in these signals due to shot-to-shot variability is less than 20%, leading to estimated errors in R of $<30\%$. At 5-ms intervals, around the time of rf heating, we used the measured plasma parameters to calculate theoretical emission line ratios. Following Sato *et al.* [25] we took the electron density to be 1.5 times the line-averaged density and the proton density to be equal to N_e. As may be seen from Table III, during rf heating (95–125 ms) our ratios compare well with observation, with discrepancies of less than 10%. From the time evolution of the radiances of the Fe XVIII lines, we can see that the intensities are at a maximum at about 120–130 ms, and are weak before and after rf heating. This could account for the large discrepancies before and after heating.

The good agreement between theory and observation provides support for the accuracy of the atomic data, both for the electron and proton excitation rates. It also implies that the theoretical results may be applied with confidence to the analysis of remote sources for which no independent estimates of N_e and T_e exist, such as solar flares.

ACKNOWLEDGMENT

V.J.F. is grateful to the Department of Education for Northern Ireland for financial support.

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