Theoretical emission line ratios for [Fe III] and [Fe VII] applicable to the optical and infrared spectra of gaseous nebulae

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Recent calculations of electron impact excitation rates and Einstein A-coefficients for transitions among the $3d^6$ levels of Fe III and among the $3d^2$ levels of Fe VII are used to derive theoretical emission line ratios applicable to the optical and infrared spectra of gaseous nebulae. Results for [Fe III] are generated for electron temperatures $T_e = 7{,}000$–$20{,}000$ K and densities $N_e = 10^2$-10^8 cm^{-3}, whereas those for [Fe VII] are provided for $T_e = 10{,}000$–$30{,}000$ K and $N_e = 10^2$-10^8 cm^{-3}. The theoretical line ratios are significantly different in some instances from earlier calculations and resolve discrepancies between theory and observation found for the planetary nebulae IC 4997 and NGC 7027.

Forbidden emission lines arising from transitions among the $3d^6$ levels of Fe III and the $3d^2$ levels of Fe VII are among the most frequently detected iron features in the high-resolution optical and infrared spectra of gaseous nebulae (1–3). Garstang *et al.* (4) and Nussbaumer and Storey (5) first pointed out the diagnostic applications of emission line ratios involving [Fe III] and [Fe VII] transitions, respectively. Subsequently, Keenan *et al.* (6) and Keenan and Norrington (7) produced updated theoretical line ratios for these ions by using electron impact excitation rates for Fe III (8) and Fe VII (9) calculated with the **R**-matrix code (10).

However, since the publication of the above papers, there have been significant improvements in the quality of the available atomic data for Fe III and Fe VII. Specifically, Nahar and Pradhan (11, 12) and Berrington *et al.* (13) have calculated improved Einstein A-coefficients and **R**-matrix electron impact excitation rates, which show large differences (of up to an order of magnitude or more) with the data adopted by Keenan *et al.* (6) and Keenan and Norrington (7). In this paper, we use the most recent atomic physics calculations for Fe III and Fe VII to derive emission line ratios for these ions over a wide range of electron temperatures and densities, for application to the spectra of gaseous nebulae.

Adopted Atomic Data. The model ion for Fe III consisted of the five LS states in the $3d^6$ ground configuration, namely ^{5}D, ^{3}P, ^{3}H, ^{3}F, and ^{3}G, making a total of 17 fine-structure levels. For Fe VII, a model ion including the five LS states in the $3d^2$ ground configuration was adopted, i.e., ^{3}F, ^{1}D, ^{3}P, ^{1}G, and ^{1}S, giving nine fine-structure levels. Energies for the Fe III and Fe VII levels were taken from Ekberg (14) and Ekberg (15), respectively.

Electron impact excitation rates for transitions in Fe III were obtained from Zhang (12), whereas those for Fe VII are from Berrington *et al.* (13). The Berrington *et al.* paper is also the source of Einstein A-coefficients for Fe VII, whereas for Fe III, the calculations of Nahar and Pradhan (11) were adopted. As discussed by, for example, Seaton (16), excitation by protons may be important for transitions with small excitation energies, i.e., fine-structure transitions. However, Reid (17) has pointed out that proton rates at low plasma temperatures, such as those considered in the present analysis, are small compared with the corresponding electron rates. Hence proton excitation is not included in the current work.

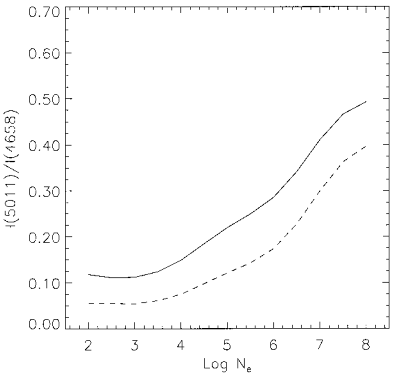

Fig. 1. Plot of the theoretical [Fe III] emission line ratio $R_1 = I(5{,}011\ \text{Å})/I(4{,}658\ \text{Å})$, where I is in energy units, as a function of logarithmic electron density (N_e in cm^{-3}) at an electron temperature of $T_e = 10{,}000$ K. The solid line shows the present calculations, whereas the dashed line is the results of Keenan *et al.* (6).

Results and Discussions

By using the atomic data discussed above in conjunction with the statistical equilibrium code of Dufton (18), relative level populations and hence emission line strengths for Fe III and Fe VII were estimated. Details of the procedures involved and approximations made may be found in Dufton (18) and Dufton *et al.* (19).

Relative line strengths for transitions among the $3d^6$ levels of Fe III [normalized to $I(4{,}658\ \text{Å}) = 1.0$] are listed in Tables 1–5, which are published as supplemental data on the PNAS web site, www.pnas.org, for a range of electron temperatures (T_e = 7,000–20,000 K) and densities ($N_e = 10^2$-10^8 cm^{-3}) appropriate to the [Fe III]-emitting regions of gaseous nebulae. Results are provided only for the strongest predicted emission lines; however, line ratios involving additional transitions, or at other values of T_e and N_e, are available from F.P.K. on request. Similarly, in Tables 6–10, which are published as supplemental data on the PNAS web site, we provide relative line strengths for transitions among the $3d^2$ levels of Fe VII [normalized to $I(5{,}721\ \text{Å}) = 1.0$] for values of temperature (T_e = 10,000–30,000 K) and density ($N_e = 10^2$-10^8 cm^{-3}) applicable to the [Fe VII]-emitting zones of nebulae. Given errors of typically ±20% and ±10% in the adopted electron excitation rates and A-values, respectively, we estimate that our derived theoretical line ratios in Tables 1–10 should be accurate to ±30%.

The temperature and density sensitivity of the [Fe III] and [Fe VII] line ratios is clear from an inspection of Tables 1–10.

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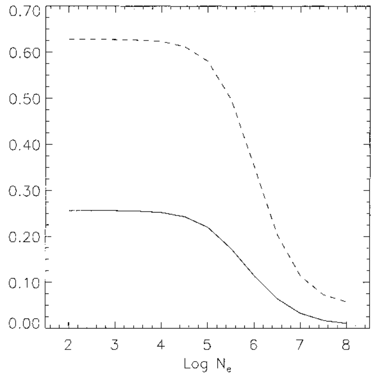

Fig. 2. Plot of the theoretical [Fe VII] emission line ratio R_2 = I(4,989 Å)/I(5,721 Å), where I is in energy units, as a function of logarithmic electron density (N_e in cm^{-3}) at an electron temperature of T_e = 20,000 K. The solid line shows the present calculations, whereas the dashed line is the results of Keenan and Norrington (7).

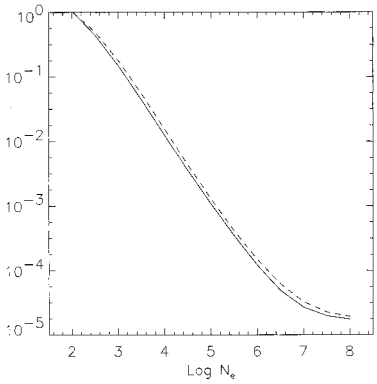

Fig. 3. Plot of the theoretical logarithmic [Fe III] emission line ratio R_3 = I(4,986 Å)/I(4,658 Å), where I is in energy units, as a function of logarithmic electron density (N_e in cm^{-3}) at an electron temperature of T_e = 10,000 K. The solid line shows the present calculations, whereas the dashed line is the results of Keenan *et al.* (6).

However, to illustrate how these results differ from those of Keenan *et al.* (6) and Keenan and Norrington (7), in Figs. 1 and 2 we plot as a function of electron density the [Fe III] ratio $R_1 = I(5{,}011\ \text{Å})/I(4{,}658\ \text{Å})$ at T_e = 10,000 K and the [Fe VII] ratio $R_2 = I(4{,}989\ \text{Å})/I(5{,}721\ \text{Å})$ at T_e = 20,000 K. The present diagnostics differ by up to a factor of 3.1 from those of Keenan *et al.* (6) and Keenan and Norrington (7) because of the adoption of improved atomic data (especially for electron impact excitation rates) in the current analysis.

We note that the present diagnostics are in better agreement with observations than previous calculations, as illustrated by the R_1 and R_2 ratios in Figs. 1 and 2, respectively. For example, Hyung *et al.* (1) measured R_1 = 0.142 for the planetary nebula IC 4997 from high-resolution echelle spectra. Adopting T_e = 10,000 K for this nebula (1) implies $\log N_e \simeq 4.0$ from the present diagnostic calculations in Fig. 1, in good agreement with both other [Fe III] density estimates ($\log N_e$ = 4.3; ref. 20) and those derived from additional lowly ionized species, such as [Cl III] ($\log N_e$ = 4.3; ref. 21). By contrast, the theoretical R_1 line ratios of Keenan *et al.* (6) imply $\log N_e \simeq 6.0$.

Similarly, Keyes *et al.* (2) determined R_2 = 0.228 from a high-resolution echelle spectrum of the planetary nebula NGC 7027. For an electron density $\log N_e$ = 4.7 appropriate to the [Fe VII]-emitting region of the nebula (22), the observed value of R_2 implies $T_e \simeq$ 19,000 K from the results in Tables 6–10. This is in excellent agreement with the temperature deduced for NGC 7027 from other high-ionization species such as [Ne IV] (T_e = 18,200 K; ref. 22). By contrast, the R_2 calculations of Keenan and Norrington (7) indicate $T_e <$ 8,000 K.

We also find good agreement between theory and observation for [Fe III] line ratios in the spectra of H II regions (23, 24). For example, Esteban *et al.* (23) have measured $R_3 = I(4{,}986\ \text{Å})/I(4{,}658\ \text{Å})$ = 0.029 for the Orion Nebula. Adopting T_e = 10,000 K for this object (23) implies $\log N_e \simeq 3.7$ from the present diagnostic calculations, shown in Fig. 3. This is in good agreement with electron densities derived from other lowly ionized species in the Orion Nebula, such as [S II] ($\log N_e$ = 3.6; ref. 23).

The above examples provide support for the accuracy and reliability of the present theoretical results. They may therefore be applied with confidence to the analysis of the optical and infrared spectra of gaseous nebulae.

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