Fe iii EMISSION LINES IN THE OPTICAL SPECTRUM OF THE PLANETARY NEBULA IC 4997

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Received 1992 October 2; accepted 1992 December 11

ABSTRACT

Relative populations for the 17 fine-structure levels in the 5D, 4P, 3H, 4F, and 3G states of the 3d6 configuration in Fe iii, calculated using electron impact excitation rates determined with the R-matrix code, are used to derive theoretical electron temperature and density sensitive emission-line ratios applicable to the spectra of astronomical objects in the 4607–5412 Å wavelength range. A comparison of these with high spectral resolution observational data for the planetary nebula IC 4997 reveals generally good agreement between theory and observation. This provides experimental support for the accuracy of the theoretical ratios, and illustrates their usefulness in determining plasma parameters for the Fe iii emitting region of a gaseous nebula.

Subject headings: atomic data — planetary nebulae: individual (IC 4997)

1. INTRODUCTION

Garstang, Robb, & Rountree (1978) first noted the diagnostic applications of emission-line ratios involving transitions among the 3d6 states of Fe iii, and presented relative line strengths determined using electron impact excitation collision rates calculated with the R-matrix code of Burke & Robb (1975). More recently, Berrington et al. (1991) recalculated these collision rates using an updated version of the R-matrix code and found some results significantly different from those of Garstang et al. For example, at T_e = 10000 K, the Berrington et al. rate for 5D_4^-3H_6 is a factor of 3 larger than that of Garstang et al., while for the 5D_4^-3D_3 transition there is a difference of 40%. These discrepancies are due partly to Berrington et al. allowing for the variation of collision strength with energy, particularly in resonances (which account for the 40% enhancement in the 5D_4^-3D_3 rate), and partly to an error in some of the collision strengths tabulated by Garstang et al.

Keenan et al. (1992) subsequently used the Berrington et al. (1991) atomic data to derive Fe iii level populations for a wide range of electron temperatures and densities applicable to astrophysical plasmas. In this paper we show how these populations may be employed in conjunction with the Einstein A-coefficients of Garstang (1957) to provide useful electron temperature and density diagnostics for the Fe iii emitting region of a plasma, and illustrate their usefulness through a comparison with high spectral resolution observations of the planetary nebula IC 4997.

2. THEORETICAL RATIOS

Level populations for Fe iii have been calculated by Keenan et al. (1992) for a wide range of electron temperatures and densities applicable to astrophysical plasmas. In their calculations these authors adopted a model ion consisting of the five LS states in the 3d6 configuration, namely, 5D, 4P, 3H, 4F and 3G, making a total of 17 fine-structure levels. The only atomic processes considered were collisional excitation and deexcitation by electrons and spontaneous radiative deexcitation, and the plasma was assumed to be optically thin. Further details of the procedures involved in the calculations and the approximations made may be found in Keenan et al. (1992).

We have used the level population results of Keenan et al. (1992) in conjunction with the Einstein A-coefficients of Garstang (1957) to derive Fe iii emission-line ratios through the well-known expression

\[ R = \frac{I(\lambda_{ij})}{I(\lambda_{mn})} = \frac{N_j A_{ji} \lambda_{ij}}{N_m A_{mn} \lambda_{mn}}, \tag{1} \]

where \( \lambda_{ij} \) and \( I(\lambda_{ij}) \) are the wavelengths and intensities (in energy units) of the lines, respectively, \( N_j \) and \( N_m \) are the upper level populations of the relevant transition and \( A_{ji} \) and \( A_{mn} \) are the Einstein A-coefficients. In Figures 1–7 we plot the ratios

\[ R_1 = \frac{I(5D_4^-3H_4)}{I(5D_4^-3D_3)} \frac{I(4987 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_2 = \frac{I(5D_5^-3P_2)}{I(5D_4^-3F_4)} \frac{I(5270 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_3 = \frac{I(5D_4^-3F_2)}{I(5D_4^-3D_3)} \frac{I(4778 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_4 = \frac{I(5D_2^-3F_3)}{I(5D_4^-3F_4)} \frac{I(4734 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_5 = \frac{I(5D_4^-3H_4)}{I(5D_4^-3D_3)} \frac{I(4881 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_6 = \frac{I(5D_2^-3F_3)}{I(5D_4^-3F_4)} \frac{I(4702 \, \text{Å})}{I(4658 \, \text{Å})}, \]

\[ R_7 = \frac{I(5D_2^-3P_3)}{I(5D_4^-3F_4)} \frac{I(5011 \, \text{Å})}{I(4658 \, \text{Å})}, \]

as a function of logarithmic electron density at electron temperatures of 5000, 10,000, 15,000, and 20,000 K. An inspection of the figures reveals that all of the ratios vary with \( N_e \), with \( R_1 \) showing the largest sensitivity, changing by a factor of 500 between \( N_e = 10^2 \) and \( 10^9 \) cm\(^{-3}\). In addition, \( R_1 \) is the ratio least sensitive to changes in the electron temperature. For example, increasing \( T_e \) from 5000 K to 10,000 K leads to only 5% and 12% decreases in \( R_1 \) at \( N_e = 10^2 \) and \( 10^9 \) cm\(^{-3}\), respectively. Hence, \( R_1 \) should in principle be exceedingly useful as an \( N_e \)-diagnostic for the Fe iii emitting region of a gaseous nebula. Unfortunately, the other line ratios (\( R_2 \),\( R_3 \),\( R_4 \),\( R_5 \)) show a significant variation with \( T_e \), so that the electron temperature would need to be known before they could be employed as reliable \( N_e \)-diagnostics. In addition, \( R_3 \),\( R_4 \),\( R_5 \) do not increase or decrease monotonically with \( N_e \), all three reach a maximum (or minimum) in the density interval \( N_e \approx 10^4 \) to \( 10^6 \)

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3. OBSERVATIONAL DATA

The observational data were secured with the Hamilton echelle spectrograph at the coude focus of the 3 m telescope at Lick Observatory during two observing runs in 1990 August 2–4 and 1991 August 30–September 1. The echelle grating, which is ruled with 316 grooves cm⁻¹ to achieve the best possible match with a CCD detector, permits coverage of the wavelength range 3600–10,300 Å. Each order contains only a small segment of the spectrum, and these are separated with the aid of a pair of low dispersion prisms which serve as cross dispersers.

The field of the 800 × 800 TI CCD is too small to cover the whole spectrum, and a complete spectral survey of a given planetary nebula requires about six chip settings. The data we have utilized here were secured in the context of a spectral survey of several planetary nebulae of high surface brightness. Among them, IC 4997 and NGC 6572 were given high priority (Feibelman, Aller, & Hyung 1992; Hyung, Aller, & Feibelman 1992). For nebular observations, a slit width of 640 μm (1:16) and a slit length of 4" were selected, giving a spectral resolution of ~0.6 Å (FWHM). These choices are imposed by constraints on spectral purity (for slit width) and overlapping orders, especially in the red (for slit length). The total area accepted by the slit is much smaller than the whole nebular image. In addition to the usual exposures on laboratory arcs and appropriate

![Graph showing theoretical Fe III emission line ratio R₁ against logarithmic electron density (Ne) at different electron temperatures (Tₑ).]

![Graph showing theoretical Fe III emission line ratio R₂ against logarithmic electron density (Ne) at different electron temperatures (Tₑ).]

... cm⁻³. Hence one would need to know the density regime of the plasma in question before applying these diagnostics. This could be achieved using, for example, the R₁ ratio.

In Figures 8 and 9 we plot R₁ against R₂, and R₁ against R₇, respectively, for a grid of (log Nₑ, Tₑ) values, where Nₑ = 10⁵–10⁶ cm⁻³ and Tₑ = 5000–20,000 K. An inspection of the figures reveals that measurements of both R₁ and R₂, or R₁ and R₇, should allow the electron temperature and density of the Fe III emitting region of the plasma to be determined, in contrast to the situation when the ratios are used by themselves, so that only Tₑ or Nₑ may be estimated.

We note that several Fe III line ratios involve transitions from common upper levels, so that they are independent of the adopted electron temperature and density, and depend only on the ratios of the A-values of the relevant transitions. These ratios, and their theoretical values, are

\[ R₈ = I(\ell^3 D₂⁻→F₄)/I(\ell^3 D₄⁻→F₄) = I(4755 \, Å)/I(4658 \, Å) = 0.180 \]
\[ R₉ = I(\ell^3 D₃⁻→F₃)/I(\ell^3 D₄⁻→F₃) = I(4769 \, Å)/I(4702 \, Å) = 0.318 \]
\[ R₁₀ = I(\ell^3 D₄⁻→F₃)/I(\ell^3 D₃⁻→F₃) = I(4607 \, Å)/I(4702 \, Å) = 0.144 \]
\[ R₁₁ = I(\ell^3 D₂⁻→F₂)/I(\ell^3 D₄⁻→F₂) = I(4778 \, Å)/I(4734 \, Å) = 0.486 \]
\[ R₁₂ = I(\ell^3 D₁⁻→F₂)/I(\ell^3 D₃⁻→F₂) = I(5412 \, Å)/I(5270 \, Å) = 0.093 \]
Fig. 3.—The theoretical Fe III emission line ratio $R_3 = \frac{I(D_{1}-D_{3})}{I(D_{2}-D_{3})}$, where I is in energy units, plotted as a function of logarithmic electron density ($N_e$ in cm$^{-3}$) at electron temperatures of $T_e = 5000$ K (solid line), 10,000 K (dashed line), 15,000 K (dotted line), and 20,000 K (dashed-dotted line).

Fig. 4.—The theoretical Fe III emission line ratio $R_4 = \frac{I(D_{1}-D_{3})}{I(D_{2}-D_{3})}$, where I is in energy units, plotted as a function of logarithmic electron density ($N_e$ in cm$^{-3}$) at electron temperatures of $T_e = 5000$ K (solid line), 10,000 K (dashed line), 15,000 K (dotted line), and 20,000 K (dashed-dotted line).

4. RESULTS AND DISCUSSION

As noted in § 2, the ratios $R_8-R_{12}$ involve transitions that are from common upper levels, so that they should always have values equal to the ratios of the relevant Einstein A-coefficients, unless the lines are optically thick and/or blended. It is highly improbable that the Fe III lines discussed in the present paper are optically thick, as they are all forbidden transitions with very small A-values ($\leq 1.0$). Hence a comparison between the observed and theoretical $R_8-R_{12}$ ratios should allow us to investigate the accuracy of the observational data, and the possible importance of blending.

An inspection of Table 1 and the theoretical values of comparison stars, one also needs a diffuse continuous source to allow for sensitivity variations from one pixel to another.

The great range in nebular line intensities imposed severe limitations on the observations. Some of our Fe III lines fall near the O III $\lambda 5007$ feature, which is $\sim 10^4$ times stronger. The long dwell times required to record features such as the faint Fe III lines result in a large oversaturation of pixels irradiated by the 5007 Å line. These saturated pixels leak along the cross dispersion direction into adjacent orders, where their effects must be evaluated. Procedures for reducing the observations are described in detail by Hyung et al. (1992). In Table 1 we summarize the observed Fe III line intensity ratios for both the 1990 and 1991 data sets. We estimate that these data should be accurate to approximately $\pm 30\%$.

To illustrate the quality of the observations, we plot in Figure 10 the wavelength region containing the strongest Fe III line (4658 Å), while in Figure 11 we plot the additional lines 4987 and 5011 Å. A high spectral resolution, such as that provided by the Hamilton Echelle, is required to separate the enormously strong ($I \approx 400$) O III $\lambda 5007$ line from Fe III $\lambda 5011$, which as noted previously is a factor of $\sim 10^4$ times weaker ($I \approx 0.04$).
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**TABLE 2**

<table>
<thead>
<tr>
<th>Ratio</th>
<th>1990</th>
<th>1991</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T_e$</td>
<td>$\log N_e$</td>
</tr>
<tr>
<td>$R_8$, $R_9$</td>
<td>7000 K</td>
<td>3.9</td>
</tr>
<tr>
<td>$R_8$, $R_7$</td>
<td><em>A</em></td>
<td><em>A</em></td>
</tr>
<tr>
<td>$R_8$, $R_7$</td>
<td>4.5</td>
<td>5.0</td>
</tr>
<tr>
<td>$R_8$, $R_7$</td>
<td>5.0</td>
<td>4.0</td>
</tr>
</tbody>
</table>

* *Indicates that the observed Fe III line ratios are larger than the theoretical limit.*

Note that a decrease in $R_3$ of only $\sim 30\%$ would lead to an electron density estimate similar to that deduced from $R_1$–$R_2$. Similarly, the $R_4$ ratio from the 1990 spectrum implies $\log N_e \approx 5.0$, while for 1991 the ratio is $\sim 25\%$ greater than the theoretical limit, and needs to be decreased by a factor of 2 to give $\log N_e \approx 4.0$. Blending of the 4734 Å line is probably the cause of this discrepancy, although the species responsible for this is not clear.

Finally, the $R_6$ and $R_8$ ratios in the 1990 spectrum, and the former in the 1991 observations, all imply $\log N_e \approx 4.0$, although $\log N_e \approx 6.0$ from $R_6$ in the latter data set. However

**Fig. 5.—** The theoretical Fe III emission line ratio $R_8 = I(4481 Å)/I(4658 Å)$, where $I$ is in energy units, plotted as a function of logarithmic electron density ($N_e$ in cm$^{-3}$) at electron temperatures of $T_e = 5000$ K (solid line), 10,000 K (dashed line), 15,000 K (dotted line), and 20,000 K (dashed-dotted line).

$R_8$–$R_{12}$ in §2 reveals good agreement between theory and experiment for $R_8$, with discrepancies of only $\sim 10\%$ for the 1990 and 1991 observations, providing support for the accuracy of the 4755 and 4658 Å line intensity measurements. Similarly, the discrepancies between the observed and theoretical results for $R_8$ are $\sim 31\%$ (1990) and $\sim 25\%$ (1991), while for $R_{11}$ the differences are $\sim 11\%$ (1990) and $\sim 22\%$ (1991), indicating that the 4769, 4734, and 4778 Å lines are relatively unblended. However the observed values of $R_{10}$ and $R_{12}$ are both at least factors of $\sim 1.7$ larger than one would expect from theory, implying that the 4607 and 5412 Å lines are probably blended, possibly with N II 4607 and Fe II 45413, respectively.

It is clear from Figures 1–9 that the best Fe III diagnostics are $R_1$–$R_2$ and $R_1$–$R_3$ in Figures 8 and 9, respectively, as they allow both $N_e$ and $T_e$ to be derived simultaneously. The observed $R_1$ and $R_3$ ratios from Table 2 imply $\log N_e$, $T_e$ = (3.9, 7000 K) and (3.8, 7000 K) for the 1990 and 1991 observations of IC 4997, respectively. In contrast, the measured $R_1$ and $R_3$ ratios lie well outside the $(\log N_e$, $T_e$) grid in Figure 9. This discrepancy could be removed by reducing the intensity of the 5011 Å line by about a factor of 2 (for the 1990 observations) and 40% (1991), implying that this transition is probably blended, possibly with N II 5011.

Adopting a value of $T_e = 7000$ K from the $R_1$–$R_2$ diagnostic, the observed $R_3$ ratio then implies $\log N_e \approx 4.5$ for the 1990 spectrum of IC 4997, with the 1991 observations lying just above the theoretical limit. However in the case of the latter we

**Fig. 6.—** The theoretical Fe III emission line ratio $R_8 = I(4470 Å)/I(4658 Å)$, where $I$ is in energy units, plotted as a function of logarithmic electron density ($N_e$ in cm$^{-3}$) at electron temperatures of $T_e = 5000$ K (solid line), 10,000 K (dashed line), 15,000 K (dotted line), and 20,000 K (dashed-dotted line).
the plasma parameters (log $N_e$, $T_e$) of the Fe III emitting region of a gaseous nebula, such as a planetary or H II region. In addition, these parameters may subsequently be used in conjunction with the line intensities to determine the iron abundance of the nebula. This is of particular importance, because in H II regions or low- and medium-excitation planetary nebulae, Fe III is often the only ionization stage of iron present in the visible spectrum and hence is the main tool for determining this element's abundance (see, for example, Clegg, Peimbert, & Torres-Peimbert 1987). However, we stress the need for high spectral resolution observational data being employed in the analysis, to reduce or remove the effects of blending on the intrinsically weak Fe III emission features.

We are grateful to A. E. Kingston for his continued interest in this work. E. S. C. and G. A. W. N. are grateful to the SERC for financial support. This work was supported by NATO travel grant 0469/87, the Nuffield Foundation, and National Science Foundation Grant AST-9014133 to the University of California, Los Angeles.

Fig. 7.—The theoretical Fe III emission line ratio $R_1 = I(D_{5}^3P_1)/I(4658 \, \AA)$, where $I$ is in energy units, plotted as a function of logarithmic electron density ($N_e$ in cm$^{-3}$) at electron temperatures of $T_e = 5000$ K (solid line), 10,000 K (dashed line), 15,000 K (dotted line), and 20,000 K (dashed-dotted line).

Once again a decrease of only $\sim 30\%$ in $R_0$ would give log $N_e \approx 4.0$.

The results of the above analysis are summarized in Table 2. An inspection of the table reveals that the electron densities deduced from $R_1 - R_0$ are in quite close agreement, especially for the better quality 1990 observational data, for which the individual values of log $N_e$ differ by typically less than 0.3 dex from the mean estimate (log $N_e = 4.3$). In addition, we note that log $N_e$ is in very good agreement with the electron densities derived from emission line ratios in other lowly-ionized species, such as S II and Cl III, which imply log $N_e = 4.0 - 4.6$ (Stanghellini & Kaler 1989).

Hyung & Aller (1992) have derived a two-component model for IC 4997, which consists of a hot, dense shell ($T_e \approx 11,000$ K; $N_e \approx 10^7$ cm$^{-3}$) of inner radius 0.0005 pc and outer radius 0.000565 pc, surrounded by a cooler, lower density ($T_e \approx 8800$ K; $N_e \approx 10^6$ cm$^{-3}$) region of outer radius 0.0013 pc. Our analysis would appear to indicate that the Fe III emission lines are formed in a zone where the temperature and density are close to those in the outer shell of the Hyung & Aller model.

The above results provide observational support for the accuracy of the Fe III diagnostic calculations, and hence the atomic data adopted in their derivation. In particular, the $R_1 - R_0$ diagnostics in Figures 1–8 may be used to infer

Fig. 8.—Plot of the theoretical Fe III emission line ratio $R_1 = I(D_{5}^3H_4)/I(D_{5}^3H_3) + I(D_{5}^3H_2)/I(D_{5}^3H_3)$ against $R_2 = I(D_{5}^3P_1)/I(D_{5}^3P_0)$ against $R_3 = I(D_{5}^3P_1)/I(D_{5}^3P_0)$, where $I$ is in energy units. The ratios are plotted for a grid of (log $N_e$, $T_e$) values, where log $N_e = 2 - 6$ in steps of 0.5 dex ($N_e$ in cm$^{-3}$), and $T_e = 5000$, 10,000, 15,000, and 20,000 K. Grid points of constant $T_e$ are connected by solid lines, while those of constant $N_e$ are connected by dashed lines.
Fig. 9.—Plot of the theoretical Fe III emission-line ratio $R_i = [I(^1D_x, ^3H_j) + I(^3D_x, ^1H_j)]/I(^3D_x, ^3F_j) = I(4987 \, \text{Å})/I(4658 \, \text{Å})$ against $R_i = R(^1D_x, ^3P_j)/R(^3D_x, ^3F_j) = I(5011 \, \text{Å})/I(4658 \, \text{Å})$, where $I$ is in energy units. The ratios are plotted for a grid of $(\log N_e, T_e)$ values, where $\log N_e = 2-6$ in steps of 0.5 dex ($N_e$ in $\text{cm}^{-3}$) and $T_e = 5000, 10,000, 15,000$ and $20,000 \, \text{K}$. Grid points of constant $T_e$ are connected by solid lines, while those of constant $N_e$ are connected by dashed lines.

Fig. 10.—Plot of the spectrum of IC 4997, observed on 1991 August 31, in the wavelength interval 4629–4660 Å. The emission lines observed in the spectrum, including Fe III 4658, are marked with laboratory wavelengths.
Fig. 11.—Plot of the spectrum of IC 4997, observed on 1991 August 30, in the wavelength interval 4982–5015 Å. The Fe III $λ4987$ and $λ5011$ lines are marked, while O III $λ5007$ is grossly overexposed. The blip near 5000 Å is due to leaking of overexposed pixels at O III $λ4959$ Å in the adjacent order.

REFERENCES