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IONIZATION STRUCTURE AND SPECTRA OF IRON IN GASEOUS NEBULAE

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RESUMEN

Presentamos un estudio de los espectros de emisión y la estructura de Fe I-IV en nebulosas gaseosas. El trabajo incluye: (I) nuevos datos atómicos; (II) estudio de los mecanismos de excitación de lineas de [Fe II], [Fe III] y [Fe IV] y análisis espectroscópico de espectros observados; (III) estudio de la estructura física y cinemática de nebulosas y sus frentes de ionización. El análisis espectroscópico de la nebulosa Orión se lleva a cabo como caso de prueba. Se muestra que la emisión de [Fe II] de Orión es excitada predominantemente por colisiones electrónicas en regiones densas parcialmente ionizadas. Evidencia adicional sobre las regiones densas es derivada de medidas de las velocidades del flujo en la nebulosa. El modelaje de fotoionización tambien indica que la emisión en el óptico de [O I] y [Fe II] se origina en regiones densas dentro del frente de ionización.

ABSTRACT

We present a study of the emission spectra and the ionization structure of Fe I–IV in gaseous nebulae. This work includes: (I) new atomic data; (II) a study of excitation mechanisms of [Fe II], [Fe III], and [Fe IV] lines, and spectroscopic analysis of observed spectra; (III) a study of the physical structure and kinematics of nebulae and their ionization fronts. Spectral analysis of the Orion nebula is carried out as a test case. It is shown that the [Fe II] emission from Orion is predominantly excited via electron collisions in high density partially ionized zones; radiative fluorescence is relatively less effective. Further evidence for high density zones is derived from measured velocities of the flow in the nebula. Photoionization models also indicate that the optical [O I] and [Fe II] emission originates in high density regions within ionization fronts.

Key Words: **ATOMIC PROCESSES — H II REGIONS — ISM: ABUNDANCES — ISM: INDIVIDUAL (ORION NEBULA) – ISM: STRUCTURE — STAR: FORMATION**

1. INTRODUCTION

The spectra, ionization structure, and the abundance of iron are valuable indicators of the physical conditions and the chemical evolution of astrophysical objects. First, owing to its relatively high abundance and the complex atomic structure of Fe ions, a large number of spectral lines are observed across most of the electromagnetic spectrum. Secondly, several ionization stages of iron may be observed from different zones within the same object. The low ionization stages of iron, Fe I–IV, generally span the physical and the ionization structure of gaseous nebulae, from the cool neutral regions and partially ionized zones, to the fully ionized regions close to the ionizing source. For instance, since the ionization potentials of Fe I and Fe II are 7.6 and 16.2 eV respectively, compared with 13.6 eV for H I, the Fe II spectrum commonly traces the conditions in partially ionized regions and ionization fronts where Fe II is shielded by H I. Thus, a combined study of Fe I–IV should provide detailed information on the structure and physical conditions of the H II region. Thirdly, while iron is primarily formed in the interstellar medium (ISM) by supernovae, it is a refractory element and its gas phase abundance constrains both the chemical enrichment of the ISM and the formation of dust grains.

The Orion nebula is commonly used as a "benchmark" for nebular studies. The present work studies the ionization structure and spectra of Fe I-IV in Orion based on: (i) new calculations of atomic data for Fe I-IV, (ii) study of ionization balance, excitation mechanisms, and radiative transfer of the spectra of Fe ions; (iii) study of the physical structure of nebulae including density and temperature variations and kinematic effects.

Despite the importance of low ionization stages of iron in laboratory and astrophysical plasmas, accurate atomic data for these ions were not available until the recent advances by the Iron Project (hereafter-IP; Hummer et al. 1993). A review of the atomic data is presented in Bautista & Pradhan (1998; BP98 hereafter).

Excitation mechanisms for iron spectra are of particular interest. Bautista, Pradhan, & Osterbrock (1994) found that the optical [Fe II] emission in Orion seems to be excited in regions with high electron densities of $\sim 10^5 - 10^7$ cm^{-3}. Further, (Bautista & Pradhan 1995a) presented evidence that [Fe II] emission in Orion stems from partially ionized zones (PIZs), where hydrogen and oxygen are mostly neutral, and collisionally excited [O I] lines are observed. At about the same time Lucy (1995) showed that the [Ni II] emission in Orion and the circumstellar nebula P Cygni could be excited by fluorescence via the background UV continuum, and suggested that [Fe II] optical emission may be similarly affected by UV fluorescence. However, Bautista, Peng, & Pradhan (1996; BPP hereafter) concluded that owing to the differences in the atomic structure, fluorescence excitation is less effective for [Fe II] than for [Ni II] and appeared relatively unimportant for Orion. Baldwin et al. (1996; B96 hereafter) argued that the UV lines of Fe II that dominate the photoexcitation are optically thick and by including self-shielding, a process not considered in BPP, the observed [Fe II] spectra could be reproduced at electron densities of $\sim 10^4$ cm^{-3}. The collisional and fluorescent excitation, including optical depth effects, are further investigated herein (§2.1).

In §2.2 and §2.3 we investigate the excitation of [Fe III] and [Fe IV] lines.

The role of kinematics in the structure of photoionized nebulae is also investigated. In diffuse H II regions the ionizing radiation from hot stars drives a strong pressure gradient that results in a stratification of velocities and ionization states of the emitting ions. This effect is discussed in § 4. In §5, some discrepancies between the predictions of current static photoionization models and the observed structure of nebulae are pointed out. Photoionization models of Orion, taking into account the high density ionization fronts are presented together with the predicted spectra of neutral and low ionization species, e.g., O I and Fe II.

2. ANALYSIS OF THE IRON EMISSION SPECTRA

We have constructed an 159-level model for Fe II. BPP discussed that, unlike the case of Ni II (Lucy 1995) where all levels participating in fluorescent excitation have the same spin multiplicity (doublets), photoexcitation of Fe II is a relatively inefficient mechanism and the critical densities for fluorescence of most lines are only of the order on 10^4 to 10^5 cm^{-3} for the radiation field in Orion. This is because the ground state of Fe II is ^6D, while most of the observed lines involve the quartet multiplets. Thus, photoexcitation of quartet levels occurs via intercombination transitions which are much weaker than the dipole transitions in low-ionization species where relativistic spin-orbit mixing is weak.

B96 have suggested that the UV lines dominating the pumping are optically thick and this would affect fluorescent excitation. For the present calculation we include optical depth effects by means of the escape probability approximation. We find the only transitions that can be considered as optically thick, $\tau > 1$, are 3 dipole allowed transitions that involve the ground state of the ion. Other transitions, most of them intercombination transitions which dominate the radiative cascades, exhibit optical depths $\lesssim 0.2$.

A sample of the [Fe II] line ratios is shown in Figs. 1. The calculated line ratios with and without optical depth effects for the UV lines are nearly indistinguishable. Therefore, optical depth effects under the conditions in Orion have negligible effects on optical [Fe II] lines. Secondly, the present results confirm earlier works (e.g., Bautista, Pradhan, & Osterbrock 1994 and BPP) showing that the optical [Fe II] line ratios are consistent with high densities ($10^5 - 10^7$ cm^{-3}). This is particularly the case for line ratios unaffected by fluorescence, which

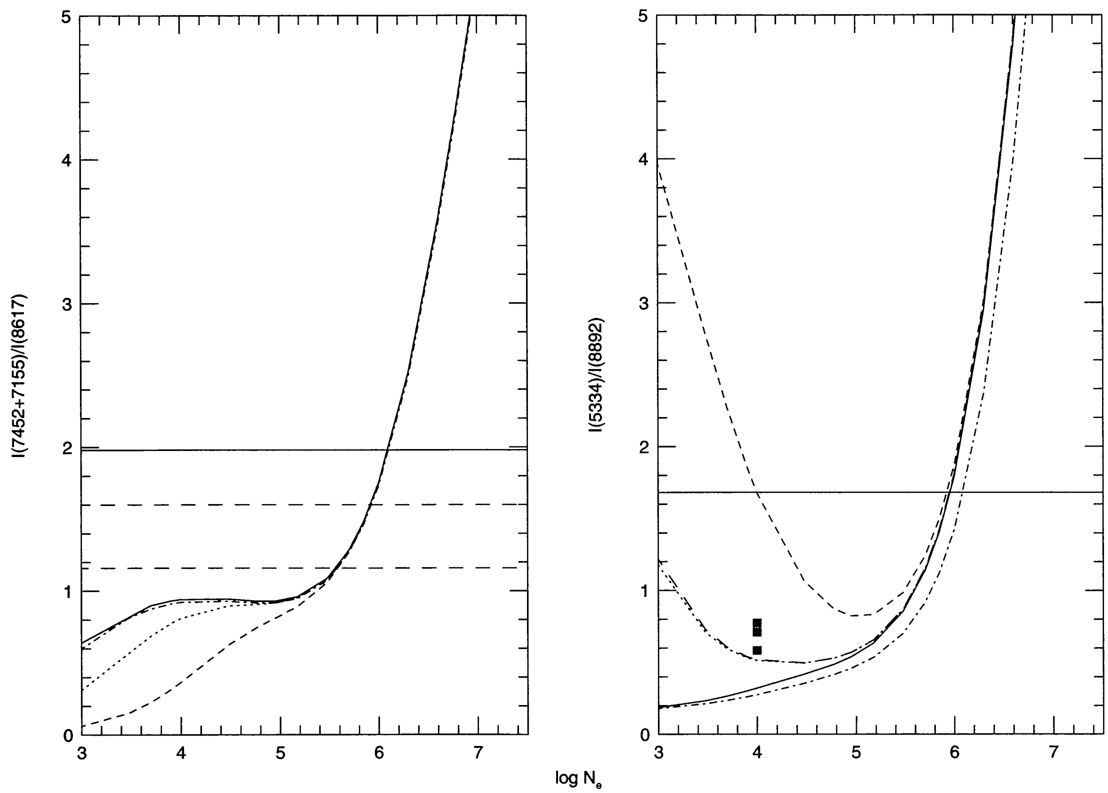

Fig. 1. [Fe II] line ratios vs. $\log N_e$ (cm^{-3}) for T_e = 10,000 K. The different curves represent pure collisional excitation (solid), collisional and fluorescent excitation without optical depth effects (dotted), collisional and fluorescent excitation including line self-shielding (long dashed), and collisional and fluorescent excitation for a UV field ten times that in Orion (short dashed). Collisionally excited line ratios calculated with collision strengths of the present 23CC calculation (short-dash and dot curves) are also shown. The predicted line ratios by Baldwin et al. (1996) are indicated by square dots. The horizontal lines indicate the observed values by OTV (solid) and Rodríguez (1996; dashed lines)

at $N_e = 4000$ cm^{-3} would yield line ratios different from the observations by more than a factor of two. Most of the line ratios from the present model agree reasonably well with the models presented by B96. Yet, both our present fluorescent model and those of B96 fail to reproduce the observed line ratios.

Additional evidence against fluorescence of Fe II in Orion is the absence of allowed emission lines in the observed spectra. If the population of the levels were dominated by cascades from the odd parity levels, the allowed transitions that result from these cascades should be seen. That is the case of the 5169.0 Å ($z\ ^6P^o_{7/2} - a\ ^6S_{5/2}$), to give an example. Then, the strength of this line should be directly related to the strength of the 4287 Å ($^6S_{5/2} - ^6D_{9/2}$) feature and, in Orion, the intensity of the 5169.0 Å line should be about 70% of that at 4287 Å. Nonetheless, no allowed Fe II lines has been observed in Orion.

We use a 34-level CR model for Fe III. One interesting characteristic of the Fe III system is that the near-IR emission originates from higher excitation levels than the optical lines which explains why the near-IR [Fe III] emission is usually very weak in gaseous nebulae. Also, the maximum energy difference between the levels that give rise to the optical lines is only about 0.02 Ry ($\sim$ 3000 K), which makes the relative line intensities of these lines insensitive to small temperature variations. Line ratios among [Fe III] lines are shown in BP98. The observed [Fe III] line ratios in Orion agree well with the diagnostics using lines of other species, such as [S II], that indicate N_e of a few times 10^3 cm^{-3}.

We use a 33-level CR model of Fe IV. Emission lines in the optical which comes from levels at about 0.5 Ry ($\sim$ 6.8 eV) above the ground state, are expected to be weak unless relatively high densities and/or temperatures are present. We identify the strongest [Fe IV] transitions for conditions of $N_e = 4000$ cm^{-3} and $T_e = 9000$ K. These UV transitions, in decreasing order of intensity, are: 2835.7 Å ($^6S_{5/2} - ^4P_{5/2}$), 2829.4 Å ($^6S_{5/2} - ^4P_{3/2}$), 2567.6 Å ($^6S_{5/2} - ^4D_{5/2}$), and 2567.4 Å ($^6S_{5/2} - ^4D_{3/2}$). Rubin et al. (1997) reported the detection of the [Fe IV] 2835.7 Å line in Orion. From this they derived the Fe/H abundance ratio in Orion to be lower than the solar by a factor between 70 and 200. A reexamination of this result is presented BP98.

In the optical region the strongest [Fe IV] features are those at 4906.6 Å($^4G_{11/2} - ^4F_{9/2}$), 4900.0 Å($^4G_{9/2} - ^4F_{7/2}$), 4903.1 Å($^4G_{7/2} - ^4F_{7/2}$), 4198.2 Å($^4G_{11/2} - ^2H_{9/2}$), and 4152.3 Å($^4G_{9/2} - ^2H_{11/2}$). However, the strength of the 4906.6 Å line with respect to the 2835.7 UV feature in Orion is only about 0.014.

Strong optical [Fe IV] emission is seen in planetary nebulae with symbiotic cores like M2-9 (Torres-Peimbert & Arrieta 1996). The reason for this seems to be the high N_e ($\sim 10^7$ cm^{-3}) in the nebular core.

3. KINEMATIC ANALYSIS OF THE ORION NEBULA

Although photoionization models generally assume static conditions, the differential expansion of nebulae is known. For example, Kaler (1967) presented radial velocities for a variety of ions taken from spectroscopic observations of Orion by Kaler, Aller, & Bowen (1965). This study includes the expansion velocity of Fe^+ obtained from [Fe II] lines. Fehrenbach (1977) reported additional measurements of three different positions in Orion which included the velocities from forbidden emission of Fe II, Ni II, and S II. The most recent kinematic studies of Orion have been presented by Castañeda (1988), Castañeda, & O'Dell (1987), and Wen, & O'Dell (1995; and references therein). In particular, O'Dell & Wen (1992) measure the expansion velocities with the [O I] λ6300 line for several arcminutes across the core of the nebula. Fig. 12 in BP98 shows the measured expansion velocities of various ions against the energy necessary to form them.

This figure reveals the dependence of the velocities of the ions on their formation energies. In particular, there is a sharp division in velocity between ions that require photon energies greater than 13.6 eV (1 Ry) and neutrals and ions with lower first ionization potentials, such as O^0, Fe^+, and Ni^+. It is also clear that forbidden emission from O I, Fe II, and Ni II should stem mostly from the same PIZ at the ionization front, as seen from the [O I]/ [Fe II] and the [Ni II]/[Fe II] correlations (BP95; BPP). The velocities associated with [S II] emission, on the other hand, lie in between those of the ionization front and the fully ionized zone. This is because, although S^+ can survive to photons up to 23.3 eV. By contrast, Fe^+ ionizes to Fe^{++} at 16.2 eV and, in addition, Fe^+ ionizes to Fe^{++} by charge exchange with H^+. Furthermore, spectroscopic diagnostics from [S II] may not agree with the [Fe II] ratios.

It is also shown that the velocities of species in the PIZ are similar to those of the photodissociation region (PDR) and the molecular cloud. From the observed velocities and using the mass conservation equation one gets a heliocentric velocity for the ionization front of about 26.6 km s^{-1}. Then,

$$\rho_{PIZ} = 10^5 \ \mathrm{cm}^{-3} \times \frac{(26.1\mathrm{kms}^{-1} - 26.6\mathrm{kms}^{-1})}{((25.8 \pm 0.6)\mathrm{kms}^{-1} - 26.4\mathrm{kms}^{-1})} \geq 4 \times 10^4 \ \mathrm{cm}^{-3}, \quad (1)$$

where 10^5 cm^{-3} is the estimated density of the PDR (Tielens & Hollenbach 1985) and 26.1 km s^{-1} is the flux averaged velocity of the PDR measured from radio C II emission (Goudis 1982). Therefore, the averaged density of the PIZ should be at least ten times greater than that of the FIZ.

4. PHOTOIONIZATION MODELING OF ORION

The new atomic data for Fe I–V enable an accurate calculation of the ionization structure of Fe. Apart from the atomic data, the main source of uncertainty in calculating the ionization structure of Fe in nebulae is the assumed structure for the cloud. Different assumptions about the radial density dependence (constant, exponential, or power law), or constant thermal and/or radiative pressure, constant temperature, etc. result in significant differences in the ionization structure of Fe and other ions. For instance, Baldwin et al. (1991) assumed a mean gas density for Orion of $\sim 10^4$ cm^{-3}, and constant gas pressure, and obtained Fe ionic fractions averaged over line-of-sight of ($Fe^+/Fe^{2+}/Fe^{3+}$) = (0.01/0.24/0.74). On the other hand, Rubin et al. (1991b) used an exponential density profile, as a function of radius, up to a maximum of 5000 cm^{-3} and a "plateau" beyond, to obtain (0.05/0.41/0.53). One might therefore expect an uncertainty of about a factor of five in an iron abundance estimate based on [Fe II] lines and ionization corrections from photoionization models. If [Fe III] lines are used instead, the uncertainty would be about a factor of two. Rubin et al. (1997) have recently estimated the iron abundance in Orion from [Fe IV] lines and obtained values that differ by nearly a factor of 3 from those of Baldwin et al. and Rubin et al. (1991b).

Another difficulty with modeling the ionic fraction of Fe^+, is the inadequacy of the physics of ionization fronts in photoionization models that assume static conditions. However, real photoionization fronts are highly dynamic and more realistic models of H II regions should consider the effect of ionization fronts where enough ionizing photons are available to photoionize new neutral material. One should also take into account the radiation energy that accelerates the gas away from the ionization front into the fully ionized zone. Not taking into account these effects results in large uncertainties in regards to the the size of the ionized region and the location of the ionization front, as can be noticed by comparing the Rubin et al. (1991a) and the Baldwin et al. models. The model of Rubin et al. uses an exponentially increasing gas density with a peak value of 5000 cm^{-3} and predicts a distance to the He ionization front of 0.277 pc. By contrast, the estimated mean thickness of the emitting region from the surface brightness of the Hα emission is only 0.13 pc (Wen & O'Dell 1995). The Baldwin et al. model, on the other hand, gives a thickness for the ionized region of about 0.07 pc, closer to observations, but the adopted density is $\sim 10^4$ cm^{-3}. Such a density is considerably higher than what is observed over most of the nebula except for a region immediately south-southwest of the Trapezium.

In modeling the ionization structure of Orion we constructed a simple model of the nebula that uses a constant density of 4000 cm^{-3}, based on long established [S II] and [O II] line diagnostics, up to a maximum distance from the star where a high density ionization front is encountered. The position of the front is optimized to match the observed relative intensity of the [O I] 6300 Å line with respect to Hβ without significantly affecting the intensities of [O II] and [O III] lines. Two models were calculated for peak particle densities of the ionization front of 10^6 cm^{-3} and 10^7 cm^{-3}. There is no explicit control over the electron density, temperature, and depth of the PIZ, and they are calculated in the model according to photoionization-recombination equilibrium. The results are presented in detail in BP98. These results reveal the difficulty in reproducing the observed spectrum with current photoionization models and, in particular, the problems in trying to simultaneously match all of the observed ionization stages of a given element, e.g., oxygen. Models like those of B96 and Baldwin et al. (1991) systematically overestimate the intensity of [O II] and [O III] from a few percent to over a factor of two. On the other hand the [O I] emission is underestimated by up to a factor of three. Both [O II] and [O III] are better modeled by adopting a mean electron density of $\sim$ 4000 cm^{-3} determined by the spectroscopic diagnostics. However, this causes the discrepancies for the [O I] lines to increase to a factor of five or more. This is because lowering the mean density increases the ionization, reducing the fractions of neutrals. Such difficulty with the neutral ion can be solved by introducing a high density PIZ at the position of the ionization front.

5. SUMMARY AND CONCLUSIONS

The physical processes of spectral formation and photoionization are described in the light of new atomic data for Fe I–IV that for reliable spectroscopic analysis and modeling of these ions. The study of forbidden optical emission spectra of [Fe II] reveals fluorescence as relatively inefficient and optical depth effects to be generally negligible. The [Fe II] emission from H II regions like Orion originates largely in high density partially ionized zones (PIZ's) within the ionization front. This conclusion is supported by nearly every line ratio among [Fe II] lines. Moreover, under fluorescent excitation the optical [Fe II] emission should be accompanied by observable dipole allowed Fe II lines. Unlike the optical emission, the [Fe II] near-IR and IR lines can be easily excited at low N_e, while they are collisionally de-excited at the high densities in the PIZ. These lines should therefore originate from a region that extends within the lower density FIZ.

The [Fe III] emission lines are primarily collisionally excited, and the observed line ratios are consistent with the conditions (T_e and N_e) of the FIZ. Optical [Fe IV] lines have been identified in only a handful of objects indicating unusually high electron densities up to 10^7 cm^{-3} and a high degree of ionization of the plasma.

There is a distinction in the observed expansion velocities for different species and their degree of ionization. Moreover, the expansion velocities of optical emission from O^0, Fe^+, and Ni^+ are remarkably similar to those of the PDR and the molecular core. This also provides evidence for the high densities in the PIZ. Similar kinematic analysis of other H II regions is proposed.

Photoionization modeling of Fe emission in Orion with the new atomic data indicates that the main source of uncertainty is the assumed structure, for example the assumption of static conditions and an *ad hoc* density profile. Particularly problematic is the region near and within the ionization front where neutrals and ions with low first ionization potentials emit.

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