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GRAINS IN IONIZED NEBULAE. II. HEAVY-ELEMENT DEPLETION

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ABSTRACT

The presence of grains in gaseous nebulae can have significant effects on the thermal balance and radiative line transfer in these objects. The depletion of condensable elements onto grains provides evidence that dust exists in the ionized regions of nebulae. In this paper, we consider the elements Sc, Ti, V, and Cr, all of which are strongly depleted in the general interstellar medium. We construct simple three-level atoms for several ions of these elements, and incorporate them into our photoionization code CLOUDY. For both a model planetary nebula and a model H II region, we find that several lines of these elements should be easily detectable, provided that their gas-phase abundances are solar. This suggests that these elements are strongly depleted in ionized regions of these nebulae. We quantify these expectations by defining and comparing line ratios which are relatively insensitive to stellar and nebular parameters with recently measured intensities of [V IV], [Cr IV], and [Cr V] lines in NGC 7027. We encourage both further theoretical and observational work on these ions.

Subject headings: atomic processes — dust, extinction — ISM: abundances

1. INTRODUCTION

Although it is well known that dust grains exist in the outer, neutral regions of gaseous nebulae, there is considerably more debate over their presence in the hotter, ionized regions. The depletion of condensable elements onto grains can provide indirect evidence for the existence of dust (see Kingdon, Ferland, & Feibelman 1995, hereafter KFF; Gaskell, Shields, & Wampler 1981; Shields 1975). Furthermore, differences in depletion determined this way for different ionization stages of a given element can suggest the presence of "depletion gradients." These, in turn, may provide a clue to the spatial distribution of the dust in these objects. Depletion gradients have been proposed for Mg (Péquignot & Stasińska 1980) and Ca (KFF).

The elements Sc, Ti, V, and Cr are all strongly depleted in the general interstellar medium (ISM). Recent estimates for the depletion are, respectively, −2.3 dex (Snow & Dodgen 1980), −2.1 dex (Crinklaw, Federman, & Joseph 1994), −2.2 dex (Cardelli 1994), and −2.2 dex (Cardelli et al. 1991). Depletions in the ISM are often strongly correlated with density. Of these four elements, this is especially true for Ti, the gas-phase abundance of which may vary by 3 orders of magnitude (Crinklaw et al. 1994).

We have recently extended our photoionization code CLOUDY to include all ions and atoms of the first 30 elements. Using the best available atomic data, we have constructed simple three-level model atoms for several ions of Sc, Ti, V, and Cr, and have incorporated them into the code. We have run two nebular models, one for a sample planetary nebula (PN) and one for a sample H II region, setting the gas-phase abundances of these four elements to solar in both cases. The results of these models can serve as a rough guide to the expected intensity of Sc, Ti, V, and Cr lines in the nondepleted case. To quantify the expectations produced by these simple models, we have run a large grid of photoionization models covering a wide range of hydrogen density and stellar temperature. We identify line ratios which are insensitive to stellar and nebular parameters and suggest that these ratios can be used as abundance indicators.

Recently, Baluteau et al. (1995, hereafter BZMP) obtained high-resolution spectra of the well-studied PN NGC 7027, down to an unreddened detection limit of 10^{-5} $I(\mathrm{H}\beta)$. They identify several lines of Ti, V, and Cr. To our knowledge, this is the first detection of these elements in PNs. By comparing the line intensity ratios predicted by the grid described above to the observed ratios from this work, we can estimate the amount of depletion of these elements.

In § 2, we discuss the model atoms, including the appropriate references for the atomic data. We also detail the parameters of our photoionization models. We present the abundance-sensitive line ratios and derive depletions for V and Cr in NGC 7027. Finally, we discuss our results and their ramifications for dust in ionized nebulae in § 3.

2. CALCULATIONS

2.1. *Model Atoms*

As stated above, we have recently added data for all of the first 30 elements to CLOUDY. Photoionization cross sections were taken from Verner & Yakovlev (1995), recombination coefficients were interpolated along isoelectronic sequences, and charge transfer cross sections were obtained from Kingdon & Ferland (1996). The dominant uncertainty in the ionization calculations is the lack of low-temperature dielectronic recombination rates. Tests suggest an error of ∼30% due to this (Ali et al. 1991).

Our first step was to construct simple model atoms for all ions of Sc, Ti, V, and Cr predicted to be abundant in gaseous nebulae. We considered only the three lowest terms of each ion, ignoring fine structure. All energy levels used were obtained from the compilation by Sugar & Corliss (1985). Next, we calculated the wavelengths of all transitions between the terms. For the purpose of this paper, we shall only consider those lines which lie in the optical or infrared.

Outside of energy levels, atomic data on these ions are generally scant or incomplete. We were able to obtain transition probabilities for most lines from Wiese, Smith, & Miles (1969); however, for a few transitions no data were

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available. In these cases, we assumed reasonable values for the transition probabilities by comparison with similar transitions in other ions.

The situation for collision strengths is considerably worse, as no data for these elements exist. We have therefore made the simplifying assumption that $\Omega_{ab}/g_a = 1$ for all lines considered, where Ω_{ab} is the collision strength between levels a and b, and g_a is the statistical weight of level a. This approximation is generally accurate to $\simeq 0.5$ dex. We note here that none of these lines are significant coolants, and so their intensity will scale directly with their atomic abundance and the collision strength. Therefore, if the collision strength for a given line as calculated above is Ω_{est}, while the actual collision strength is Ω_{true}, the true abundance of the element will simply equal the abundance derived here times the ratio $\Omega_{\text{true}}/\Omega_{\text{est}}$. The uncertainty in the collision strengths will be the dominant error in what follows.

2.2. *Models*

The atomic data described in the previous section have been incorporated into CLOUDY, a self-consistent photoionization code which maintains both ionization and thermal balance. More extensive details on the code can be found elsewhere (Ferland et al. 1997).

In order to get some idea of the intensities of Sc, Ti, V, and Cr lines in gaseous nebulae, we have run two sample models. The first is the standard Paris PN model (Ferland et al. 1995). This model considers a gas of typical nebular abundances, with a constant hydrogen density of 3000 cm^3 s^{-1}, ionized by a 150,000 K blackbody. We note that many refractory elements are depleted, but grains are not included in the model. The second model is an H II region, based on the Orion Nebula (Baldwin et al. 1991). This model uses typical H II region abundances and Orion grains. The total pressure is kept constant, and the hydrogen density is 10,000 cm^3 s^{-1} at the ionized face. The gas is ionized by a 39,700 K star (Kurucz 1991). Further details of these models can be found in Ferland (1993). In both models, the abundances of Sc, Ti, V, and Cr were set to solar values (Grevesse & Anders 1989).

We present our results in Table 1, which lists the intensities of several multiplets with respect to Hβ. We note here that the intensities are for the total multiplet; the individual line intensities will be appropriately smaller. As is apparent from this table, several lines of Ti, V, and Cr should be readily observed in nebulae, provided that these elements have solar gas-phase abundances.

TABLE 1

MODEL LINE INTENSITIES

Ion	Wavelength (Å)	PN Intensity	H II Intensity
Ti III	12100	3.6(−3)	8.8(−3)
Ti III	9594	9.2(−4)	1.7(−3)
V III	8823	3.5(−4)	8.6(−4)
V IV	7735	3.2(−4)	3.2(−4)
V IV	9489	1.7(−3)	8.2(−4)
Cr IV	7267	6.7(−2)	2.4(−2)
Cr IV	6801	2.8(−2)	9.0(−3)
Cr V	7979	6.6(−2)	4.0(−4)
Cr V	6577	1.0(−2)	...
Cr V	37400	1.4(−2)	...

NOTE—All intensities are with respect to $I(\text{H}\beta) = 1.0$. The notation $a(b)$ here means $a \times 10^b$.

In order to quantify these results, we make use of the observations of BZMP, who identified and measured intensities for several lines of [V IV], [Cr IV], and [Cr V] in the well-studied PN NGC 7027. Rather than develop a detailed photoionization model for this object, we shall take the approach used by KFF; namely, we will identify line ratios which are insensitive to nebular or stellar parameters, but which depend on the abundances of the ions in question.

To assist in this goal, we have computed a grid of over 200 photoionization models. Although this grid is somewhat coarser, it is essentially identical to the PN grid discussed in KFF. The models consider a constant density gas, ionized by a blackbody, and having a filling factor equal to unity. The reader is referred to KFF for more details. For convenience, we list in Table 2 the abundances adopted for all elements, as some of these differ from the KFF grid. The abundances listed for Sc, Ti, V, and Cr are solar values.

For each [V IV], [Cr IV], and [Cr V] multiplet for which BZMP list an intensity, we used the results of the grid to construct line intensity ratios that depend only weakly on stellar and nebular parameters, as discussed above. We chose the following five intensity ratios: [V IV] λ7735/N II λ5680, [Cr IV] λ6801/[O III] λ5007, [Cr IV] λ7267/[O III] λ5007, [Cr V] λ6577/[Fe V] λ3892, and [Cr V] λ7979/[Fe V] λ3892. For each ratio, we may write an equation like

$$\left[\frac{V}{N}\right]\bigg/\left[\frac{V}{N}\right]_{\odot} = g(n_{\text{H}}, T_*) \times \frac{I(7735)}{I(5680)}\,, \qquad (1)$$

where the term on the left-hand side represents the abundance ratio relative to solar. As discussed above, for our chosen five intensity ratios, the function $g(n_{\text{H}}, T_*)$ will be only weakly dependent on its parameters. Thus, by comparing the predicted values of these ratios with those observed, we can derive depletions for these elements. We discuss each of these ratios and the resulting depletions below.

We present our chosen line intensity ratios graphically in Figure 1, which depicts contour plots of each ratio as a

TABLE 2

MODEL ABUNDANCES

Element	Abundance
He	0.10
C	7.8(−4)
N	1.8(−4)
O	4.4(−4)
Ne	1.1(−4)
Na	3.0(−7)
Mg......	1.6(−6)
Al	2.7(−7)
Si	1.0(−5)
S	1.0(−5)
Cl	1.7(−7)
Ar.......	2.7(−6)
Ca	1.2(−8)
Sc	1.23(−9)
Ti	8.6(−8)
V........	1.05(−8)
Cr.......	4.84(−7)
Fe.......	5.0(−7)
Ni.......	1.8(−8)

NOTE—The notation $a(b)$ here means $a \times 10^b$. Abundances for the first 30 elements not listed here were set equal to 1.0(−9).

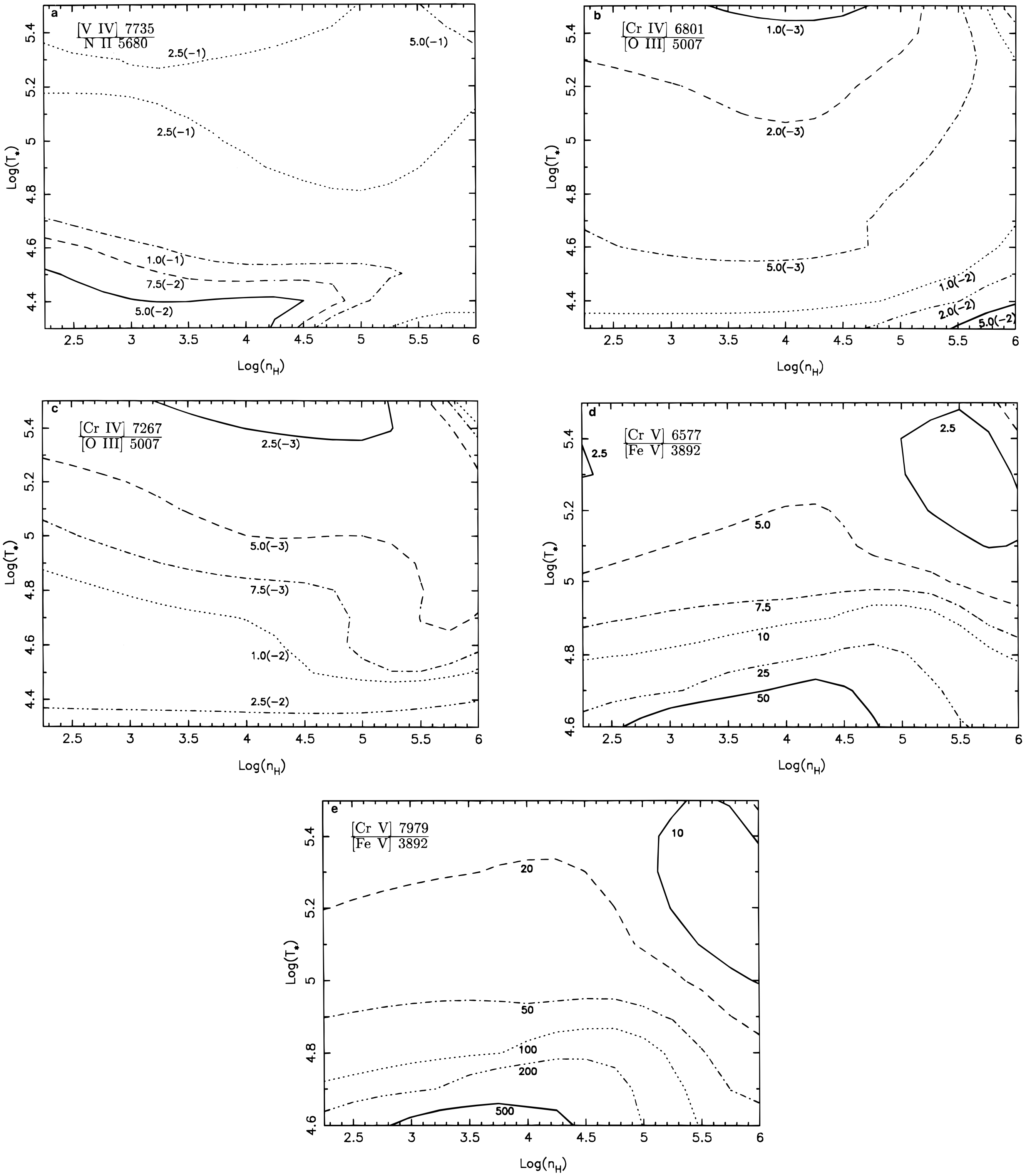

FIG. 1.—Contour plots of various line ratios as functions of central star temperature (T_*) and total hydrogen density ($n_{\rm H}$). The line ratios are as follows: (*a*) [V IV] λ7735/N II λ5680; (*b*) [Cr IV] λ6801/[O III] λ5007; (*c*) [Cr IV] λ7267/[O III] λ5007; (*d*) [Cr V] λ6577/[Fe V] λ3892; (*e*) [Cr V] λ7979/[Fe V] λ3892.

function of total hydrogen density ($n_{\rm H}$) and stellar temperature (T_*). The range in T_* is less in Figures 1*d* and 1*e*, as our models suggest that the ionization is insufficient to produce one or both ions in the line ratio. As is readily seen, these ratios are relatively insensitive to $n_{\rm H}$ and T_* over a wide range of parameter space. We may quantify this in the following way. Consider reasonable observational uncertainties of 0.25 dex in $n_{\rm H}$ and 0.2 dex in T_*. We then determine the resulting uncertainty in the line intensity ratio at several points in the grid and average these values. For the five ratios depicted in Figure 1, this average uncertainty is 37%, 45%, 44%, 62%, and 66%, respectively.

We may now compare the results of Figure 1 with observation to estimate depletions. Since BZMP's data are longward of 6540 Å, we have also used the observations of Keyes, Aller, & Feibelman (1990) of NGC 7027 to form the appropriate line ratios. The two data sets were scaled by strong lines common to both sets, which have minimum observational uncertainty and no telluric absorption. The resulting line intensity ratios were then corrected for reddening using a logarithmic extinction at Hβ c = 1.37. Finally, each [V IV], [Cr IV], and [Cr V] line intensity was converted to its multiplet intensity under the assumption that all fine-structure levels are populated according to their statistical weight. In order to compare with the grids, we shall take log $n_{\rm H} = 4.7$–4.85, and log $T_* = 5.24$–5.3 for NGC 7027 (see Keyes et al. 1990; Middlemass 1990; Gruenwald 1989).

We present our results in Tables 3 and 4. Table 3 provides the observational data. Column (1) lists the line ratio considered. Columns (2) and (3) give the observed intensity ratio uncorrected for reddening, and after correction, respectively. Finally, column (4) gives the factor by which the line intensity must be multiplied in order to convert to the multiplet, as explained above.

TABLE 3

OBSERVED LINE RATIOS

Line Ratio (1)	$F^{\rm a}_{\rm Ratio}$ (2)	$I^{\rm b}_{\rm Ratio}$ (3)	Correction Factor (4)
[V IV]λ7742 / N II λ5680	3.81(−1)	1.57(−1)	4.55
[V IV]λ7857 / N II λ5680	4.10(−1)	1.69(−1)	2.56
[Cr IV]λ6896 / [O III]λ5007	1.38(−5)	5.22(−6)	6.67
[Cr IV]λ6915 / [O III]λ5007	1.08(−5)	4.08(−6)	1.92
[Cr IV]λ7391 / [O III]λ5007	7.65(−6)	2.45(−6)	2.94
[Cr V]λ6710 / [Fe V]λ3892	2.75(−1)	4.58(−2)	2.70
[Cr V]λ7884 / [Fe V]λ3892	7.40(−1)	8.46(−2)	1.59

NOTE—The notation $a(b)$ here means $a \times 10^b$.

[a] Flux ratio before correction for reddening.

[b] Reddening-corrected flux ratio.

The results of Table 3 are then used in Table 4 to derive the depletions. Here column (1) lists the line intensity ratio used in determining the depletion, while column (2) gives the wavelength of the observed member of the multiplet used from BZMP. The observed intensity of the ratio (obtained by multiplying the values in cols. [3] and [4] of Table 3) is given in column (3). Column (4) gives the predicted value of this ratio, based on Figure 1, and the values of the parameters for NGC 7027 given above. Finally, column (5) gives the logarithmic depletion derived from comparing columns (3) and (4).

3. DISCUSSION

Before discussing the interpretation of our results from the previous section, we must first examine the source and size of the uncertainties in these results. The uncertainties in our predicted line ratios due to uncertainties in the nebular and stellar parameters have already been discussed. We will therefore begin with the observational uncertainties. The errors in the [V IV], [Cr IV], and [Cr V] line intensities used here were estimated by BZMP to range from 10% to 60%. The correction for reddening introduces additional uncertainty. We have tried to minimize this effect when possible by choosing line ratios in which the two wavelengths differ by relatively small amounts. Still, we estimate an average uncertainty due to reddening of ∼70% in the observed line intensity ratios, with larger uncertainties for larger wavelength differences, and vice versa. A relatively small uncertainty results from the scaling of the BZMP spectra to that of Keyes et al. (1990).

The major source of uncertainty in our results stems from the lack of accurate atomic data, especially collision strengths. It is difficult to estimate the uncertainty introduced by our $\Omega_{ab}/g_a = 1$ assumption, but factors of 0.5 orders of magnitude would not be surprising. A smaller uncertainty occurs in the conversion of the individual line intensity to the multiplet intensity, based on uncertainties in the transition probabilities and our assumption that the fine-structure levels are populated according to statistical weight. The uncertainties in our model line ratios due to uncertainties in the nebular and stellar parameters have already been discussed, and amount to ∼50%.

One final concern needs to be addressed. In our derivation of depletions of V and Cr in NGC 7027 in the previous

TABLE 4

DERIVED DEPLETIONS IN NGC 7027

Line Ratio (1)	Wavelength (2)	Observed (3)	Predicted (4)	Depletion (log) (5)
[V IV]λ7735 / N IIλ5680	7742	7.15(−1)	3.00(−1)	−0.38
	7857	4.35(−1)	3.00(−1)	−0.16
[Cr IV]λ6801 / [O III]λ5007	6896	3.48(−5)	1.78(−3)	1.71
	6915	7.85(−6)	1.78(−3)	2.36
[Cr IV]λ7267 / [O III]λ5007	7391	7.20(−6)	2.90(−3)	2.60
[Cr V]λ6577 / [Fe V]λ3892	6710	1.24(−1)	3.11(0)	1.40
[Cr V]λ7979 / [Fe V]λ3892	7884	1.34(−1)	1.60(1)	2.08

NOTE—The notation $a(b)$ here means $a \times 10^b$. A negative value in col. (5) corresponds to an enhancement rather than a depletion.

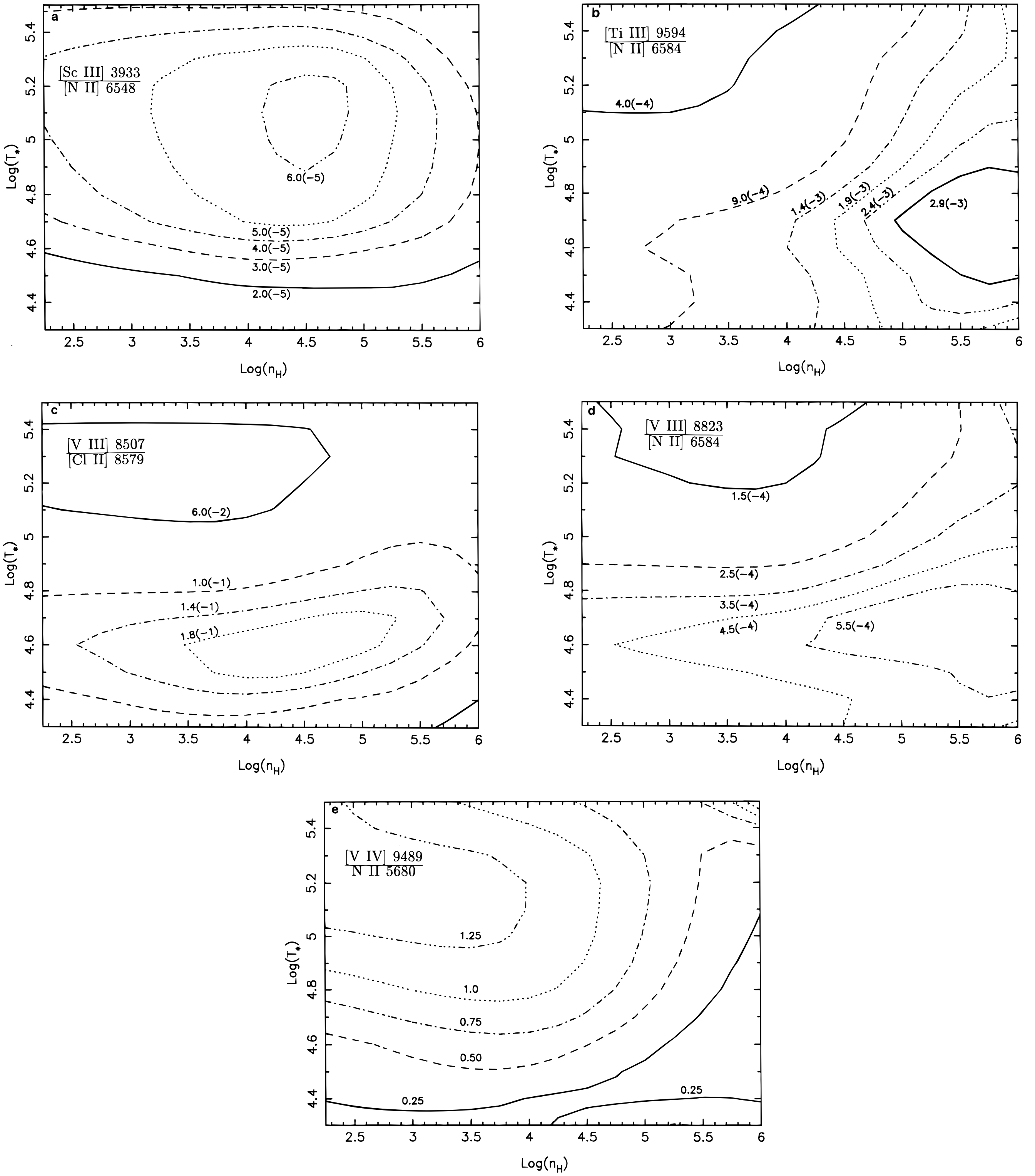

FIG. 2.—Same as Fig. 1, for the following line ratios: (*a*) [Sc III] λ3933/[N II] λ6548; (*b*) [Ti III] λ9594/[N II] λ6584; (*c*) [V III] λ8507/[Cl II] λ8579; (*d*) [V III] λ8823/[N II] λ6584; (*e*) [V IV] λ9489/N II λ5680.

section, we implicitly assumed that the difference between the observed and predicted line intensity ratios was due solely to the abundance of V or Cr, i.e., the element in the numerator. In reality, we must also consider the abundances of the elements in the denominator of the line ratios. A quick comparison between the input abundances for N, O, and Fe in Table 1 and derived abundances for these elements in NGC 7027 (see Keyes et al. 1990; Middlemass 1990) shows differences of only ∼0.15 dex for N and O, and ∼0.3 dex for Fe.

Keeping the above uncertainties in mind, we may now interpret the results of the last section. We begin with [V IV]. As shown in Table 3, BZMP observed two members of the λ7735 multiplet, and we have derived depletions (or in this case, enhancements) from both of them. The results from the two lines agree to within 60%, consistent with the quoted observational uncertainties in the line measurements. To within the uncertainties discussed in the preceding paragraphs, our results for [V IV] are consistent with no depletion, although either a mild depletion or enhancement is possible. Since [V IV] will exist between an ionization potential of ~30–50 eV, the observed lines of this ion will be formed well within the ionized zone.

We next consider [Cr IV]. BZMP observed lines of this ion from two separate multiplets. For the $\lambda 6801$ multiplet, two lines were measured. The depletions derived from these two lines of the same multiplet differ by a factor of ~4.5, far greater than the stated uncertainties in the line intensities. There are at least three possible explanations for this discrepancy: (1) the BZMP measured intensities for one or both lines are in error, or their estimated uncertainties are much too conservative; (2) the A-values for one or both lines are in error; or (3) the transitions are not in *LS*-coupling. If we average the depletions from these two lines along with that from the $\lambda 7391$ line of the $\lambda 7267$ multiplet, we obtain a depletion of roughly 2 orders of magnitude relative to solar. We believe that this depletion is real, and not simply the result of the various uncertainties. If this is indeed the case, there are several important ramifications. First, the high ionization potential of the [Cr IV] ion implies that grains do exist in highly ionized environments. Similar conclusions were reached by Shields (1975) and KFF for Fe and Ca, respectively. Second, since the [Cr IV] lines used here are formed in nearly the identical region of NGC 7027 as the [V IV] lines discussed previously, these grains must have the property of strongly depleting Cr but not V.

Finally, we consider [Cr V]. BZMP measured one line each from two multiplets of this ion. Averaging the results yields a depletion of slightly more than 1.5 orders of magnitude. If we again consider this to indicate a true depletion, these results provide evidence that grains can exist in very highly ionized (≥ 50 eV) regions. Further, a comparison of the results for [Cr IV] and [Cr V] indicates the existence of a depletion gradient, in the sense that fewer grains exist in the hotter [Cr V] zone than in the relatively cooler [Cr IV] zone. Improved data are required before it can be determined whether this is a real effect or merely the result of the uncertainties.

Clearly, much work needs to be done before the results of this paper can be stated with certainty. Better transition probabilities are needed, but the lack of collision strengths provides the major source of uncertainty here; these data are sorely needed. The observational side of the problem is much more promising. The work of BZMP has demonstrated that measurement of very weak lines in nebulae is possible with current detectors. A program with the major goal of obtaining accurate intensity measurements of heavy-element lines in nebulae would be feasible and would yield important results.

Toward this end, we present in Figure 2 additional contour plots useful in determining depletions from several other lines of Sc, Ti, V, and Cr. Lines from four of the five multiplets in Figure 2 were observed by BZMP, but no intensities were given.

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