OBSErvations of [S III] in NGC 604 and N/S Abundance Gradients*

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ABSTRACT

We have obtained line intensities for NGC 604—a giant H II region in M33—in the wavelength range 56312–10049. Observations of [S III] λλ9069, 9532 yield a S++ abundance and an accurate total S abundance in agreement with that for the Orion Nebula. Previous investigators have seriously overestimated N/S. We discuss the use of [N II]/[S II] as an abundance indicator and conclude that, while a gradient in [N II]/[S II] implies a gradient in N/S, a dependable calibration of line ratio versus abundance is unavailable.

Subject headings: galaxies: individual — nebulae: abundances — nebulae: individual

I. INTRODUCTION

Certain important emission-line ratios have been observed to show systematic variations in the H II regions across the disks of spiral galaxies; these include [O III]/Hβ, [N II]/Hα, and [N II]/[S II] (Aller 1942; Burbidge and Burbidge 1962; Searle 1971; Benvenuti, D’Odorico, and Peimbert 1973; Smith 1975; Jensen, Strom, and Strom 1976). These variations have generally been attributed to abundance gradients. However, since many physical processes affect emission-line strengths in gaseous nebulae, this interpretation is still heavily model-dependent (Peimbert 1968; Searle 1971; Benvenuti, D’Odorico, and Peimbert 1973).

In the cases where electron temperatures have been measured, the existence of abundance gradients seems clearly established. Smith (1975) observed [O III] λ4363 in three nebulae in M33 and five nebulae in M101 and was able to compute directly the O and N abundances for the outer regions of the galaxies. Hawley (1977) has found gradients in O/H and N/H based on observations of H II regions between 8 and 14 kpc from the center of our Galaxy. In other cases the ratio [N II]/[S II] has been used to deduce the N/S abundance based on a calibration similar to that given by Benvenuti, D’Odorico, and Peimbert (1973).

As yet, no study has included both the electron temperature and the relevant ionic abundances necessary to compute total O, N, and S abundances. Specifically, the emission lines of [S III] λλ9069, 9532 have not been observed because of the lack of sensitive detectors in the near-infrared. Observations of [S III] are important since S+ would not be expected to be the predominant ionization stage of S because of its rather low ionization potential (23.3 eV), and the ionization potential of N+ (29.5 eV) is sufficiently different that N+ and S+ conceivably occupy different volumes.

As part of a program under way at Lick Observatory to obtain photoelectric spectrophotometry of emission-line objects in the near-infrared, we have observed NGC 604, a giant H II region in M33. Since NGC 604 has been observed previously by Peimbert (1970), Peimbert and Spinrad (1970), and Smith (1975) in the wavelength range λλ3727–6731, we have concentrated on the spectrum between λλ6000 and λλ10000. In particular, we have measured the [S III] lines λλ9069, 9532. On the basis of these new observations we have recomputed the abundances of N and S, and have rediscussed abundance gradients in M33. We also analyze the use of [N II]/[S II] and [O III]/Hβ as abundance indicators, and of [S III] as a temperature diagnostic.

II. OBSERVATIONS

The observations were made with the Wampler sequential scanner (Wampler 1966) and the 90 cm Crossley reflector on the nights of 1976 November 16 and 17. The data were taken in the single-channel mode. The detector was a VPM-164 photomultiplier tube with an InGaAsP photocathode which is on consignment to Lick Observatory from Varian Associates. This photomultiplier tube has a spectral response from 1145 to 11,000 Å. Throughout the blue-green region of the spectrum its quantum efficiency is comparable to, or greater than, the S-20 photocathode. In the red and near-infrared the VPM-164 has 10–20 times the quantum efficiency of the S-1. Typical values are 18% at 4000 Å, 8% at 7000 Å, 3.5% at 10,000 Å, and 2% at 10,600 Å (Klein, private communication).

The entrance hole of the scanner measured 14.0. In the region from 6000 to 7000 Å we used an exit slit of 0.6 × 5 mm giving a resolution of 19.6 Å in order to resolve Hα; [N II] λ6583; and [S II] λλ6717, 6731. The bandpass containing λ6312 was centered to the red of λ6312 in order to exclude the night-sky line at λ6300. Beyond 7000 Å the resolution was 32 Å. The data were put on an absolute energy scale from observations of the standard stars γ Gem, η Hya, ε Cet, 29 Psc, and ε Aqr, which have been calibrated by Hayes (1970).
The line fluxes normalized to $F(\text{H} \alpha) = 100$ are presented in Table 1. Errors in the line intensities are approximately 20% for $F(\lambda) \geq 10$ and approximately 25%–50% for $F(\lambda) < 10$. The agreement is excellent between our data and the data of Smith (1975) and of Peimbert and Spinrad (1970) for $\left[ \text{N} \, \text{ii} \right]/\text{H} \alpha$ and $\left[ \text{S} \, \text{ii} \right]/\text{H} \alpha$. Since we did not observe H$\beta$, we adopt the logarithmic reddening correction $c(\text{H} \beta) = 0.22$ given by Peimbert and Spinrad. The reddening-corrected line intensities are also given in Table 1. We can check the reddening correction by comparing $I(\text{P}7) = 2.2$ with the theoretical value of 1.9 for $(\text{P}7 \lambda 10049)/\left(\text{H} \alpha \lambda 6563\right)$ (Brocklehurst 1971). These values are consistent, given the quoted errors in $F(\text{P}7)$.

### III. ABUNDANCES

Ionic abundances are determined from the reddening-corrected line fluxes and the following expression:

$$
\frac{X}{\text{H}^+} = \frac{\lambda \left( \text{Å} \right) \left[ S(X) N_e a(4,2; \text{H}^0) \right]}{4861 \left( P(X,n) A \right)} \frac{I(\lambda, X)}{I(\text{H} \beta)}.
$$

Equation (1)

$X/\text{H}^+$ is the relative number density of ion $X$; $P(X,n)/S(X)$ is the population of the upper state of the transition relative to the population of all levels in ion $X$; $a(4,2; \text{H}^0)$ is the effective recombination coefficient for forming H$\beta$; and $A$ is the transition probability. We calculated the ratios $P(X,n)/S(X)$ using a multilevel atom program which incorporated transition probabilities and collision strengths given by Osterbrock (1974), except that the $N^+$ and $O^+$ collision strengths came from Seaton (1975) and from Eissner and Seaton (1974), respectively.

To convert ionic abundances to total abundances, we employ the following formulae (Peimbert and Costero 1969):

$$
\frac{N}{H} = \frac{N^+ O}{H^+ O^+},
$$

Equation (2)

$$
\frac{S}{H} = \frac{S^+ + S^{++} O}{H^+ O^+}.
$$

Equation (3)

Because of the similarity in the ionization potentials of $S^{++}$, $N^+$, and $O^+$, these formulae should be quite good. The accuracy of formula (2) has been discussed previously by Hawley and Miller (1977). We have adopted $T_\text{e} = 9100 \text{ K}$ from $I(\text{H}4363)/I(\lambda 5007)$ (Smith 1975). The calculated abundances are insensitive to the value of the electron density at the density implied by $I(\lambda 6717)/I(\lambda 6731)$. We also adopt $O^+/O = 0.61$ from Smith.

Table 2 presents the ionic and total abundances from this paper, along with Smith’s abundances for NGC 604 and a recent determination of abundances in the Orion Nebula by Peimbert and Torres-Peimbert (1977). We have not used the temperature correction procedure outlined by Peimbert (1967) and by Peimbert and Costero (1969); therefore, the abundances we derive will be systematically less than if we had taken $t^2 = 0.055$ as did Smith. The abundances for the Orion Nebula from Peimbert and Torres-Peimbert were computed with $t^2 = 0.0$.

We did not observe $[\text{O} \, \text{ii}]$ or $[\text{O} \, \text{iii}]$, but the O abundance in NGC 604 as determined by Smith (1975) and by Peimbert (1970) is similar to the O abundance in the Orion Nebula. The N abundance we derive is less than that for the Orion Nebula by a factor of 2.2. We believe that this is real and that N is underabundant in NGC 604 with respect to H II regions in the solar neighborhood. Smith has already demonstrated that N/O is more than a factor of 2 lower for the outer regions of M33 than for the Orion Nebula.

The S abundance we derive is a factor of 3.3 larger than the abundance derived by Smith. This is no doubt due to the presence of $S^{++}$, which has not previously been taken into account. On the other hand, our $S^+$, $S^{++}$, and total S abundances for NGC 604 agree well with those for the Orion Nebula. Furthermore, the N/S ratio is more than a factor of 5 lower than the value that would be deduced from the observed $[\text{N} \, \text{ii}]/[\text{S} \, \text{ii}]$ and the assumption $N(N^+)/M(S^+) \approx M(N)/M(S)$. We will discuss this point in more detail below.

To summarize this section, the abundances of O and S in NGC 604 are completely typical of solar neighborhood H II regions while N is underabundant by about a factor of 2. The use of the ratio $[\text{N} \, \text{ii}]/[\text{S} \, \text{ii}]$ to determine abundance gradients must be critically examined.
IV. MODEL CALCULATIONS

The ratio \((\text{N} \text{III}) \lambda 6548, 6583) / (\text{S} \text{III}) \lambda 6717, 6731)\) has been used to obtain the ratio \(N^+ / S^+\) in a way that is insensitive to exact knowledge of the electron temperature or reddening correction. The constant adopted for proportionality between line intensity and abundance varies from author to author but can be computed for a given set of collision strengths and range of temperatures. Benvenuti, D’Odorico, and Peimbert (1973) included the assumption that \(N^+ / S^+\) is insensitive to exact knowledge of the electron temperature or reddening correction. The constant derived for the 06 V star is \(0.42\) and a filling factor of 0.04 were assumed. The base abundances used in the calculation were \(\text{He}/H = 0.12\), \(\text{Ne}/H = 1.0 \times 10^{-4}\), \(\text{C}/H = 3.0 \times 10^{-4}\), and \(\text{Si}/H = 4.0 \times 10^{-5}\).

Table 3 summarizes the models. Listed for the various abundances are the electron temperature in the middle radii of the nebula, the maximum electron temperature in the outer region of the nebula, the \([\text{O} \text{III}] \lambda 4959 + \lambda 5007\) line strength, the \([\text{S} \text{III}] \lambda 9069 + \lambda 9532\) to \([\text{S} \text{II}] \lambda 6716 + \lambda 6731\) and the \([\text{N} \text{II}] \lambda 6548 + \lambda 6583\) to \([\text{S} \text{II}] \lambda 6716 + \lambda 6737\) line ratios, and the ratio of the \(N/S\) abundance ratio to the \([\text{N} \text{II}]/[\text{S} \text{II}]\) ratio.

The models in which the \(N\) and \(S\) abundances are varied show clearly that \([\text{N} \text{II}]/[\text{S} \text{II}]\) reflects very well the \(N/S\) ratio over order-of-magnitude changes in either \(N\) or \(S\). Basically, the addition or subtraction of \(N\) or \(S\) has very little effect on the temperature or ionization structure of the outer parts of the model nebula where \(S^+, S^{++}\), and \(N^+\) exist. Since from equations (2) and (3) we can derive

\[
\frac{N}{S} = \frac{N^+}{S^+ + S^{++}},
\]

we can safely ignore the inner regions of the nebula. However, the effect of changing the \(O\) abundance is to change the electron temperature in the outer regions of the model nebula by a larger amount, which causes the proportionality constant between \(N/S\) and \([\text{N} \text{II}]/[\text{S} \text{II}]\) to increase by a factor of 1.5 for a 3000 K temperature change. This change is caused both by the variation in the \(S^{++}\), \(S^{++}\) ionization structure (as indicated by the change in \([\text{S} \text{III}]/[\text{S} \text{II}]\)) and by the different sensitivities of the \([\text{N} \text{II}]\) and \([\text{S} \text{II}]\) lines to variations in \(T_e\).

However, further model calculations show that the proportionality constant is also dependent on the assumed form of the ionizing spectrum. Models with \(O/H = 4.5 \times 10^{-4}\), \(N/H = 4.5 \times 10^{-5}\), and \(S/H = 2.0 \times 10^{-5}\) and with an ionizing spectrum representing an \(O4\) V star (50,000 K), an \(O8\) V star (35,000 K), and a \(B1\) V star (22,500 K) give proportionality constants of 0.28, 0.86, and 3.1, respectively, instead of the 0.42 constant derived for the \(O6\) V star. This change is for

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the most part caused by a variation in the S$^{++}$, S$^+$ ionization structure, as is indicated by [S iii]/[S ii] line ratios of 8.0, 9.6, 2.3, and 0.12 for the O4 V, O6 V, O8 V, and B1 V star models, respectively (of course, [S iii]/[S ii] also depends on $T_e$).

In other words, under conditions of unchanging excitation and unchanging electron temperature, a gradient in [N ii]/[S ii] reflects very reliably a change in N/S. However, the presence of gradients in $T_e$, caused mainly by an O/H gradient (Shields 1974; Smith 1975) and in excitation caused by a correlation between dust and element enrichment (Sarazin 1976), or of a variation in the temperature of the exciting stars (Shields and Tinsley 1976) seems to be essential to an acceptable theory of line gradients in external galaxies. The convolution of a presumed N/S gradient with the presumed drop in electron temperature and with the presumed softening of the ionizing spectrum from the outer to the inner H II regions of a galaxy would therefore seem to be quite complicated. However, both the $T_e$ gradient and the excitation gradient would predict a drop in [N ii]/[S ii] from the outer to the inner regions, so that the observed rise in [N ii]/[S ii] does indicate that N/S is increasing toward the center of the galaxy; but the absolute determination of a N/S gradient from the [N ii]/[S ii] gradient appears to be impossible.

Our observations of NGC 604 lead to a factor of 0.36 between N/S and [N ii]/[S ii], with a [S iii]/[S ii] line ratio of 4.5—both values well within the range predicted by the models.

Before leaving the model calculations, a mention should be made of the [O iii]/H$\beta$ line ratio. As indicated by our models, [O iii]/H$\beta$ is not a monotonic function of O/H and, furthermore, very large O/H ratios are required to bring [O iii]/H$\beta$ down below 1. This latter effect is caused by [O iii] emission from the outer radii of the nebula, where the harder radiation field causes a large rise in electron temperature (Shields 1974). The deduced softening of the stellar ionizing radiation does, however, serve to decrease [O iii]/H$\beta$ with a less dramatic increase in O/H (Sarazin 1976). In other words, analyses that utilize [O iii]/H$\beta$ as the sole indicator of heavy-element enrichment (Jensen, Strom, and Strom 1976) are heavily dependent on assumptions concerning the ionization structure of H II regions. Any reliable determination of heavy-element abundance must be based on more complete observations including a temperature determination.

V. DISCUSSION

The discussion in § IV indicates that abundances determined from [N ii]/[S ii] must be viewed with caution. Unless independent knowledge of a $T_e$ gradient or excitation gradient can be obtained, it seems that the observed gradient in [N ii]/[S ii] indicates no more than the presence of a gradient in N/S. In no case does it appear advisable to calculate magnitudes of gradients or abundances of N/S for individual nebulae from [N ii]/[S ii] alone.

We feel that we have demonstrated the necessity of having observations of [S iii] in hand before attempting to determine the magnitudes of gradients in S and N/S. An accurate S$^{++}$ abundance permits the N/S ratio to be calculated without an accurate measure of $T_e$, since ratios of abundances from forbidden lines are much less sensitive to variations in the temperature than are ratios from recombination lines. Otherwise, there appears to be little hope of obtaining N/S, since most of the S is not in the form of S$^+$ and since no straightforward way exists to calibrate a relationship between N/S and [N ii]/[S ii].

In addition, observations of [S iii] may provide the best method of determining the electron temperature in the inner extragalactic H II regions. The unavailability of temperature data is due mainly to the systematic decrease of [O iii]/H$\beta$ with decreasing distance from the nucleus. S$^{++}$ has several properties which make it a potentially useful temperature diagnostic. The ionization potential of S$^+$ is low (23.3 eV); so with much of the S in the form of S$^+$, the nebular lines should be strong. Furthermore, the ratio $I(\lambda 6312)/I(\lambda 9065 + \lambda 9532)$ is 2%—3% at H II region temperatures while $I(\lambda 4363)/I(\lambda 4959 + \lambda 5007)$ is 0.2%—0.4%. Owing to the similarity of the various ionization potentials, the [S iii] temperature is presumably representative of the region where S$^+$, O$^+$, and N$^+$ exist. For observations with modern low-resolution detectors, the night-sky lines near $\lambda 6312$ might cause a less severe problem than the mercury lines in the spectral regions around $\lambda 4363$ and $\lambda 5755$. However, the flux in $\lambda 6312$ given in Table 1 should be considered an upper limit because of the inherent weakness of the line and possible contamination by [O i] $\lambda 6300$. The corresponding upper limit to $T_e$ ([S iii]) is 11,000 K.

How do the results presented here affect the conclusions of previous investigators? The value of N/S for the inner regions in M33 derived by Benvenuti, D’Odorico, and Peimbert (1973) relies on the assumption that N$^+/S^+ = N/S$. This assumption was motivated by their observation that a plot of [N ii]/H$\alpha$ versus [S ii]/H$\alpha$ for inner H II regions could be fitted by a line with slope unity. They argued that, since the line intensities increase in direct proportion, N$^+$ and S$^+$ occupy similar volumes, which they interpreted as an implication that N$^+/N = S^+/S$. Our models, however, show that N$^+$, S$^+$, and S$^{++}$ occupy the same region of the ionized nebula, so that, presumably, a plot of [S iii]/H$\alpha$ versus [N ii]/H$\alpha$ for the same H II regions plotted by Benvenuti, D’Odorico, and Peimbert (1973) could also be fitted with a line of slope 1. In other words, their assumption must be replaced with equation (4). We do point out that the observations of Benvenuti et al. imply that [N ii]/[S ii] is a constant for the inner H II regions of M33. This result might be expected if N/S were approximately constant for these H II regions, as discussed above.

Models which predict N$^+/S^+ \approx N/S$ have been discussed by Peimbert, Rodriguez, and Torres-Peimbert (1974). They consider photoionization by a single star in a temperature range 30,000—35,000 K and find that, for very low density or very large
dilution factors, N$^+$ and S$^+$ occupy similar volumes. Whether these models more correctly describe the H II regions near the nucleus of M33 probably cannot be determined without more detailed observations.

Balick and Sneden (1976) have also computed model H II regions in which the volume where S is S$^+$ can constitute a large fraction of the N$^+$ zone. A comparison of the ratio of the various ionized volumes in one model ($T_e = 40,000$ K, $N_e = 10$, $Z = Z_0$) calculated by our program to the results in their Table 1 shows fairly good agreement for the ratios $X(N^+)/X(O^+)$, $X(O^+)/X(S^+)$, and $X(S^+)/X(S^+)$. However, the ratios $X(N^+)/X(S^+)$, $X(O^+)/X(S^+)$, and $X(S^+)/X(S^+)$ are larger in our models by factors of 10.5, 6, and 4.6, respectively. We attribute this difference to the fact that the model atmosphere used by Balick and Sneden was a local thermodynamic equilibrium (LTE) atmosphere that has a larger drop in flux at the He$^+$ ionization edge near 25 eV than does the non-LTE atmosphere used in our calculations. Therefore, our models have less S$^+$ relative to the other low-ionization species. We feel that our models are in better agreement with the observations of NGC 604 and so our models have less S$^+$ relative to the other low-ionization species. We feel that our models are in better agreement with the observations of NGC 604.

Comte's (1975) observation that [N II]/[S II] increases across M33 and M101, and Sivan's (1976) observation of a gradient in [N II]/[S II] across our Galaxy imply gradients in the N/S abundance; but nothing can be said with confidence concerning the magnitude of the gradient or whether there is an underabundance or overabundance with respect to the solar neighborhood.

The most comprehensive study of line intensity gradients across spiral galaxies remains that of Smith (1975). With O/H abundances for the outskirts of M33 and M101, the observed [N II]/[S II] gradient, and the assumption that N/S $\approx$ N/O he derived N/H gradients from edge to center. Unfortunately, without S$^{++}$ abundances the total S abundances must be considered lower limits; so whether or not O/S is constant remains unclear. Furthermore, as we have seen, the magnitude of the N/S gradient cannot easily be determined from the line intensities alone.

In summary, except for the outskirts of M33 and M101, there exists no convincing observational determination of magnitudes of abundance gradients. Model calculations do support the contention that a gradient in [N II]/[S II] implies an N/S gradient, even though an accurate calibration would be very difficult to make because the line intensity gradients are influenced by too many factors for each to be easily deconvolved. However, observations of [N II], [S II], and [S III] would allow the determination of N/S gradients in galaxies.

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